HIGH-FREQUENCY SILICON ACOUSTO-ELECTRONICS

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HIGH-FREQUENCY SILICON ACOUSTO-ELECTRONICS

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For my family and all humankind.

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A BRIEF INTRODUCTION

1.1 INTRODUCTION TO SURFACE ACOUSTIC WAVES

Surface acoustic waves (SAWs) are acoustic waves confined to the surface of a material. First described by Lord Rayleigh in 1885 [1], surface acoustic wave use has since grown to stratospheric heights today with applications in communications, sensors and fundamental physics research [2–6]. SAWs decay exponentially into the substrate they propagate on and thus, penetrate to only about one wavelength λ . The broad term for SAWs encompasses many different types of wave motions and polarizations, however, in this work we concentrate on Rayleigh waves, which are shear-vertical, longitudinally propagating surface acoustic waves [7]. An example of a SAW is shown in figure 1.1a, where the periodic vertical surface displacement is sketched along with the penetration of the wave into the substrate.

SAWs are generated with an interdigitated transducer (IDT) on a piezoelectric substrate via the inverse piezoelectric effect [8, 9]. The IDT has finger electrodes with a periodicity corresponding to the SAW wavelength λ_{SAW} which excite SAWs with a frequency f_{SAW} dependent on the SAW velocity v_{SAW} in the substrate:

$$\lambda_{SAW} = v_{SAW} / f_{SAW}. \quad (1.1)$$

Figure 1.1b shows an IDT exciting SAWs as an RF voltage is applied to it with a specific frequency f_{SAW} .

The velocity of plane acoustic waves (bulk) in non-piezoelectric materials is given by $v = \sqrt{c_{ij}^E / \rho}$, where c_{ij}^E is the elastic coefficient in the direction of propagation and ρ is the material density. In piezoelectric materials, however, the relations governing the interaction of electric fields and strain must be taken into account and the linear piezoelectric constitutive equations are [9, 10]:

$$T_{ij} = c_{ijkl}^E S_{kl} - e_{kij} E_k, \quad (1.2)$$

$$D_i = e_{ikl} S_{kl} + \epsilon_{ik}^S E_k, \quad (1.3)$$

where T_{ij} is the stress tensor, S_{kl} the strain tensor, e_{kij} the piezoelectric tensor, E_k the electric field, D_i the electric displacement field, and ϵ_{ik}^S is the permittivity of the material under constant strain.

Similarly, the wave equation in piezoelectric materials is modified with an extra term including the electric potential ϕ :

$$\sum_{j,k,l=1}^3 c_{ijkl}^E \frac{\partial^2 u_l}{\partial x_k \partial x_j} + \sum_{j,k=1}^3 e_{ijk} \frac{\partial^2 \phi}{\partial x_k \partial x_j} = \rho \frac{\partial^2 u_i}{\partial t^2}, \quad (1.4)$$

where $\mathbf{u}$ is the displacement field [11, 12]. The resulting velocity in piezoelectric media is then dependent on a linear combination of elastic and piezoelectric constants. For Rayleigh waves, the displacement field in the wave equation is $\mathbf{u} = (u_x, 0, u_z)$. A more in depth primer can be found in Ref. [13] and a thorough analytical solution for surface acoustic waves in Ref. [7, 9, 11, 14].

1.1.1 Acousto-electronic transport

Surface acoustic waves in piezoelectric media modify the semiconductor band gap in two ways. First, the type I modulation which changes minutely the band gap itself and follows the change in crystal lattice with the propagating SAW. This creates band gap maxima and minima directly corresponding to the volume change of the lattice [15]. And second, the type II modulation which changes the band gap edges through the piezoelectric field accompanying the SAW. Similar to type I, it creates traveling maxima and minima, however, without changing the band gap itself and with the additional advantage of the valence band maxima and conduction band minima being spatially separated [16]. A schematic of such SAW semiconductor interaction is shown in figure 1.1c [17].

Free charge carriers can become dragged by a SAW via the band-gap modulation in what is called acousto-electronic transport (ACT). First demonstrated in germanium by Weinreich and White in 1957 [18], ACT gained prominence in GaAs after single electron transport with SAWs was observed [19, 20], and today it has been used in transferring single electrons between distant quantum dots [21]. In the figure 1.1c, in addition to band gap modulations, photo-generated carriers are sketched as being captured and spatially separated in an example of acousto-electronic transport [17].

Acousto-electronic transport efficiency depends on sufficient free carrier mobility. A good rule of thumb is $v_{drift} > v_{SAW}$, where the carrier drift velocity is also dependent on $v_{drift} = \mu E_x$, with μ carrier mobility and E_x the piezoelectric field of the SAW [22]. However, there are more complex mechanisms of transport that may need to be taken into account outside of the condition above [23–26] and at low temperatures [27].

Figure 1.1: Surface acoustic waves and their interaction with semiconductors. a) Material surface deformation by a surface acoustic wave (SAW) with a wavelength λ , which penetrates to about one wavelength into the substrate. The image was generated in COMSOL Multiphysics and has an exaggerated vertical displacement for a better visual aid. b) An interdigitated transducer (IDT) which is used to excite SAWs by converting an electrical impulse to mechanical waves via the inverse piezoelectric effect and vice versa for detection of SAWs. c) Top: a sketch of the crystal lattice modulation via SAWs. Bottom: Modification of the band gap edges by a SAW on a semiconductor, thereby trapping charge carriers for acousto-electronic transport. Courtesy of [17].

1.2 EXPERIMENTAL METHODS

1.2.1 Fabrication

The main IDT fabrication method in this work is a UV-based nano-imprint lithography (NIL). It uses a pre-fabricated quartz template that has the desired features etched in a negative pattern. The quartz template is made using high quality e-beam at IMS Chips, Germany. Here, all the critical dimension features, such as IDT fingers and connecting bus-bars, are made in one step.

The NIL process is a step-and-flash process. Step means the template is positioned over an imprint area and then lowered into an imprint resist, thereby transferring the pattern. The flash is the hardening of the resist via UV light, after which the template is released so it can move on to another position and imprint again. This can be repeated many times until a substrate (wafer) is fully imprinted [13].

With care, a template lifetime is on the order of 10,000 imprints, if not more. The template used in this work is in service since 2012 and has been imprinted at least several thousand times.

This lithographic method has many advantages: it is substrate material independent (there are no substrate-dependent back-scattering effects as in e-beam or optical lithography), it is geared for large scale fabrication (high speed), it has a high resolution and critical dimension control (the imprint template can be produced to high quality and small feature size), and a high reproducibility as the fabrication is based on a single template.

The disadvantages are in the initial cost of the quartz template, which once produced can not be changed, therefore, the initial design process has to be thorough in debugging. Additionally, the process is incompatible with small substrates as the capillary pressure holding the template during imprinting can be prohibitive to template detachment. And finally, the imprint process is surface quality sensitive. Contaminated substrates with particles or with high total thickness variation (TTV) can impair proper template imprinting and thus pattern transfer.

An overview of the NIL process can be seen in figure 1.2 and is adapted from the work by Büyükköse et al. [28]. First, a substrate that is going to be used for NIL, unless it is out-of-box from the manufacturer, has to be thoroughly cleaned. We use a 15 to 30 minute acetone/IPA/DI water ultrasonic bath procedure. Once the substrate is prepared, a 100 nm organic transfer layer (lift-off layer) is spin coated onto the wafer (fig. 1.2a-(i)). Next, imprinting is carried out using S-FILTM with an *Imprio*TM 55 tool from Molecular Imprints, Inc. The imprinting proceeds on a field-by-field basis with each field covered prior to imprinting with an organic, UV-curable resist *Monomat*TM from Molecular Imprints, Inc. (fig. 1.2a-(ii)). The substrate is positioned underneath the imprint template and the template is pressed into the resist with a force of 2 – 3 N

Figure 1.2: UV-flash nano-imprint lithography (NIL) a) Step by step overview of the NIL process. Adapted from [28]. b) A completely imprinted 100 nm wafer after HSQ spin-coating for planarization (vi). c) IDT features with bus bar contacts after the RIE etching step (viii). d) SEM image of metallized IDTs after lift-off with feature size 80 nm (step (x)).

(fig. 1.2a-(iii)). The resist is cured and hardened via broadband UV-light at 230-320 nm wavelength (fig. 1.2a-(iv)). The template is released and lifted, leaving a positive pattern transferred onto the substrate (fig. 1.2a-(v)). The step and flash imprinting can proceed until the substrate is filled as desired.

Planarization is carried out with spin-coating of 100 nm HSQ (DC XR 1541-006 from *Dow Corning*) on top of all the imprinted features at 1,500 rpm for 30 seconds and then the substrate is baked at 150 °C for 3 minutes (fig. 1.2a-(vi)). A fully imprinted and planarized wafer is shown in fig. 1.2b. In this image, the imprints are aligned via an optical microscope during imprinting to functionalized features in the substrate.

Spin-coating the HSQ is advantageous because the HSQ thickness is lower on top of regular, periodic features, such as IDT fingers and bus-bars. This

enables the next step, the etch-back with reactive ion etching (RIE) of the HSQ with CHF_3 plasma with an Adixen AMS100DE tool. The etch-back opens up the IDT patterns of imprint resist, while leaving other empty areas covered with a residual thin layer of HSQ (~ 10 nm) (fig. 1.2a-(vii)). A second RIE step with O_2 plasma etches the imprint resist vertically down to the substrate (fig. 1.2a-(viii)). The etch selectivity of the imprint resist and transfer layer versus the HSQ is ~ 100 . A scanning electron microscope (SEM) image of a sample with an etched NIL pattern is shown in fig. 1.2c. The selectivity of the RIE is demonstrated with only slight side wall under-etch, which helps during lift-off.

Metallization is done with e-beam evaporation (BAK600) and the materials used are interchangeable. Usually a thin ($\sim 2 - 5$ nm) adhesion layer of Cr or Ti is deposited followed by a conductive Al or noble metal layer ($10 - 25$ nm) with an optional capping layer of ~ 10 nm Ti (fig. 1.2a-(ix)). Finally, the sample is dipped into an ultrasonic bath of solvent for lift-off (fig. 1.2a-(x)). Figure 1.2d shows a SEM image of an IDT fabricated via a NIL process. Seen are double finger electrodes of the IDT on the right and a bus-bar connecting them on the left.

1.2.2 Measurements

There are two NIL templates used in this work, one with single finger (SF) IDTs and one with double finger (DF) IDTs. The IDT configurations are showed in figures 1.3a and 1.3b. The finger feature sizes are 65, 80, 100, and 125 nm, corresponding to SF IDT wavelengths $\lambda = 260, 320, 400$, and 500 nm and DF IDT wavelengths $\lambda = 520, 640, 800$, and 1,000 nm [13].

The devices on the NIL template used throughout this work are delay lines (fig. 1.4a). Delay lines are two IDTs separated by a specific distance. As their name implies, they introduce a delay in a signal: an electrical signal on one IDT (port 1) is transformed to a mechanical wave with an acoustic velocity much slower than the speed of light. The mechanical wave travels the separation distance and is transformed back to an electrical signal by the second IDT (port 2).

Such delay lines can be used to assess the performance of IDTs with an equivalence to a two-port network (fig. 1.4b). The network performance is measured by a *vector network analyzer* (VNA) and evaluated with S-parameters which are complex numbers representing traveling waves in a transmission line. In the case of a two port network, the relationship between the input (a_i) and output (b_i) voltage signals during a network analysis is given by:

$$\begin{pmatrix} b_1 \\ b_2 \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}, \quad (1.5)$$

Figure 1.3: IDT designs a) Single finger (SF) IDT, where $\lambda = 4 \times p$ and p is the finger feature size. b) Double finger (DF) IDT, where $\lambda = 8 \times p$.

where S_{ii} are the reflection and S_{ij} are the transmission parameters [7, 29].

The reflection S_{11} is the ratio of the reflected to the incident signal at port 1. In principle, it is equal to S_{22} . The transmission S_{12} is the ratio of reflected signal in port 1 to the incident signal at port 2. For S_{21} , the ratio is of the reflected signal in port 2 to the incident signal at port 1. Similarly to the reflection, the transmission $S_{12} = S_{21}$. With SAW experiments, the reflection is used to see if any SAWs are being excited by an IDT and the transmission is used to check if SAWs are traveling between two IDTs, such as in a delay line.

An example of a two port S-parameter vector network analysis is shown in figure 1.4c. Reflection S_{11} shows a dip around $f_{SAW} = 3.6$ GHz, which signifies a loss of returning signal power in port 1. This loss is attributed to a conversion of electrical to mechanical energy at the IDT: SAW generation. The transmission S_{21} exhibits a peak at the same frequency as the dip in the reflection. This additional energy at port 2 is from an arriving SAW sent by the IDT at port 1, which is transformed from a mechanical wave to an electrical signal at the receiving IDT. The SAW velocity can be extracted via $v_{SAW} = \lambda \cdot f_{SAW}$.

There are many nuances in a measurement such as shown in figure 1.4c. In the reflection, the background signal level is important to gauge the level of incident power loss at the transmitting IDT. The reflection background level in fig. 1.4c is at around ~ -8.5 dB. This is quite low and can signify poor IDT resistance or even large capacitive behavior. The dip in the reflection, showing SAW generation, is also quite shallow ~ 0.5 dB, indicating low electromechanical coupling of the IDT to the substrate.

Likewise, in the transmission, the background signal level around the resonance can indicate other acoustic and EM phenomena, such as the presence of spurious (bulk) modes or EM cross-talk between the IDTs. The transmission background shown in the fig.1.4c is quite low ~ -100 dB and uniform. This

Figure 1.4: IDT configuration and measurement. a) Two IDTs placed after each other in a *delay line* with a separation distance $d = 1,085 \mu\text{m}$, which is fixed on the NIL template. b) Schematic of a vector network analysis (VNA) of a *device under test* (DUT) in a two port configuration, which yields the scattering parameters of the device. c) The scattering parameters of SAW delay line as seen in (c). Dips in the reflection S_{11} signify a loss of return signal in port 1, which is attributed to SAW generation. Peaks in the transmission S_{21} are additional energy at port 2 from arriving SAW sent by an IDT at port 1. The SAW velocity can be extracted directly $v_{\text{SAW}} = \lambda f_{\text{SAW}}$.

is due to another key feature of VNA, time-gating. Time gating can be used to decouple the SAW signal from the background, thereby enhancing it, and will be introduced more in chapter 3 and 4. The SAW transmission shown in fig. 1.4c has very low power $< -80 \text{ dB}$, even with time-gating, which means the arriving SAW is very weak, indicating problems in the propagation of the SAW.

The aspects of network analysis of delay lines and IDTs will be used in this work many times and explored into great detail for several materials.

1.3 OUTLINE OF THESIS

The goal of this study is to achieve successful application of high-frequency SAWs for acousto-electric charge transport (ACT) in silicon.

Chapter 2 starts with the introduction of a benchmark acousto-electronic transport device fabricated on a $\text{SiO}_2/\text{ZnO}/\text{SiO}_2$ multilayer on silicon substrate. Vector network analysis of the IDT delay lines used in the ACT device are compared at room temperature and at 10 K. An IV characteristic of the ACT device is also analyzed at both temperatures. Further, a triggering scheme

of the ACT measurement in the time domain is employed as an attempt to filter out the electromagnetic interference generated by the IDT.

Chapter 3 goes into detail about the piezoelectric thin-films used to fabricate ACT devices on silicon. A piezoelectric $\text{SiO}_2/\text{ZnO}/\text{SiO}_2$ multilayer on a silicon substrate is analyzed by numerous methods, both material, structural and acoustic (SAW) to gauge its suitability for ACT applications. And finally, a wet etch of the multilayer is made to test if SAW propagation is improved without the thin-films between IDTs.

In chapter 4, a comparison between free and capped single crystal lithium niobate is made to demonstrate the effect a thin film SiO_2 capping layer has on SAW propagation. The change in propagation loss due to the presence of the film is analyzed and shown also in the time domain.

In chapter 5, we numerically simulate the ZnO multilayer used in previous chapters to obtain the SAW electromechanical coupling constant. The results are applied to an IDT equivalent circuit model for electrical impedance matching to $50\ \Omega$ and then compared to the experimental IDTs used via NIL in chapter 3 and 4. An ideal IDT length (number of finger pairs) is found for impedance matching for specific SAW wavelengths and ZnO thin-film thicknesses.

In chapter 6, a novel thin-film piezoelectric, ScAlN, deposited on silicon is analyzed via SAWs generated with NIL delay lines. The thin-film SAW generation and propagation characteristics are analyzed via a VNA and compared to the multilayer in the previous ZnO chapters. The experimental IDT electromechanical coupling constant is calculated and compared to literature and numerical simulations.

And finally, chapter 7 gives an outlook into a new generation of silicon ACT devices using the knowledge and experience from the previous chapters of this thesis in their design. A new thin-film material combination and fabrication process flow is proposed to minimize damage to the piezoelectric thin-films used in potential new devices. Numerical simulation and the equivalent circuit model from chapter 5 are used to assess the ideal IDT length with the proposed new material structure. Additionally, alternate IDT designs are introduced for improved generation and propagation of high frequency SAWs with larger wavelength IDTs.

OPTO-ACOUSTO-ELECTRONIC DEVICES

2.1 INTRODUCTION

Surface acoustic waves (SAWs) are strain waves propagating along a material surface and can be excited on a piezoelectric material via an interdigitated transducer (IDT) [7]. The piezoelectric potential of SAWs modifies semiconductor band edges such that the local bandgap minima and maxima can trap and drag free charge carriers. For most fundamental acousto-electric investigations, a single-crystal piezoelectric substrate is desirable to prevent extraneous acoustic modes and deleterious SAW propagation effects. GaAs substrates, with an GaAs/AlGaAs two-dimensional electron gas 2DEG system, are explored extensively for acousto-electronic transport (ACT) applications [21, 30–32].

Silicon, on the other hand, is the main workhorse of the semiconductor industry and for quantum electronics research it is interesting for its long electron spin lifetimes. However, it is not piezoelectric and needs an additional piezoelectric layer to excite surface acoustic waves. Acousto-electronic transport in silicon was recently demonstrated at megahertz frequencies via a ZnO piezoelectric thin-film [22]. However, high frequencies (> 5 GHz) are needed for effective acousto-electronic transport and to enter the quantum regime [33].

Here, we use a nano-imprint lithographic (NIL) process to define interdigitated transducers with wavelengths from $\lambda = 1,000$ nm down to 520 nm (double-finger design with a finger width from 125 nm to 65 nm) [28]. We explore the suitability of this top-down, CMOS-compatible process with piezoelectric thin-films by fabricating silicon acousto-electronic transport devices.

We combine a series of four experiments designed to test our fabrication and thin-film material. The benchmark device is a photon detector based on previous work by Barros et. al., 2012 [22] and S. Büyükköse. In addition, we fabricate a device with an electrostatic constriction (quantum point contact - QPC) in the path of the SAW [30], an electrostatically driven switch (to attract carriers laterally), and a photon generator (based on electron-hole recombination). The latter three devices are not experimentally characterized in this work.

2.2 DEVICE STRUCTURE AND FABRICATION

An intrinsic silicon substrate (100 mm, $\rho > 10 \text{ k}\Omega \text{ cm}^{-1}$ from Sievert Wafer GmbH) is first thermally oxidized at $1,050^\circ\text{C}$ in a dry oxidation oven to grow a 100 nm film of silicon oxide. The substrate is subsequently selectively doped with boron and phosphorus via ion-implantation for p- and n-type, respectively, carrier injection and detection regions. Next, 100 nm of Wurtzite ZnO is deposited with RF magnetron sputtering (Paul-Drude-Institut für Festkörperelektronik, Berlin, see Ref. [22] for details) and capped with an additional 20 nm of sputtered SiO_2 . Nano-imprint lithography is used to fabricate Ti/Ag/Ti (5/20/5 nm) IDT delay-lines aligned to the doped silicon regions. Ohmic contacts to the doped silicon areas are opened with wet chemical etching, using BHF and highly diluted HC1 (0.5 %wt), for SiO_2 and ZnO respectively. Then Ti/Ag/Ti (5/40/20 nm) nanowires are fabricated with electron-beam lithography (EBL) for carrier injection into the SAW path and quantum point contact structures. And finally, all electrostatic structures, IDTs, and wet etched regions are contacted with Ti/Al/Ti (5/100/20 nm) electrodes using optical lithography.

Figure 2.1 shows a schematic of a photon detector device on the $\text{SiO}_2/\text{ZnO}/\text{SiO}_2/\text{Si}$ multilayer substrate. Figure 2.1b shows an optical image of such a finalized device. The principle of operation is as follows: surface acoustic waves are generated at the IDT (left in Fig. 2.1a or out of the topside of Fig. 2.1b). Traveling SAWs reach an excitation region, where a laser is generating excitons in the silicon. The excitons are captured and dragged by the SAW through a series of electrostatic gates, which separate the electron and hole of the exciton laterally. And finally, the SAWs deliver the excitons to a recombination region in the form of a p-i-n doped silicon diode. The p-i-n diode is biased in the reverse regime $V_{\text{pn}} > 0 \text{ V}$ and any additional carriers brought by the SAW into the diode depletion region will result in a frequency-dependent increase in the dark current I_{pn} [22].

The photon detector is our main benchmark device for silicon acousto-electronic transport in general, however, for single-electron transport lateral confinement is needed as well. Figures 2.2a and 2.2b show optical images of a QPC device, with features fabricated with EBL shown in SEM images below (Figs. 2.2c and 2.2d). In the optical images, the SAW is generated from an IDT on the left side of the image and captures electrons brought into its path via a lead gate (Fig. 2.2a(i)). Next, the SAW reaches the QPC, at which all dragged electrons but one are pushed back electrostatically. The SAW, now potentially dragging only a single electron per wave trough, arrives at the doped detection region (Fig. 2.2a(ii), where the carried electrons are detected as an increase in current [30].

The sputtered ZnO/ SiO_2 layers are visible in the SEM images in Figs. 2.2c and 2.2d. The polycrystalline structure of the ZnO thin-film is clearly visible

Figure 2.1: Schematic of substrate, device and function of a Si-based ACT photon detector. Left: complete device schematic, Right: optical image of the exciton generation and detection region of a finished device. The photon detector is on a ZnO/Si multilayer substrate with doped silicon regions indicated in blue (n++) and red (p++). The NIL IDT sends out a SAW, which drags excitons generated by a laser. The dragged excitons can get further spatially separated by electrostatic gates until they reach a p-i-n diode, where they can recombine and are detected. Based on design by S. Büyükköse.

along with random dark voids, which are missing grains. The film after fabrication and processing appears in quite poor condition and therefore, traveling SAWs are expected to have poor transmission.

Two additional devices are fabricated; an acousto-electronic transport switch (see Figs.2.2e and 2.2f) and a photon generator (not shown). The switch device uses a lead gate as an electron source, after which electrostatic gates, which push and pull the SAW-dragged electrons laterally in a chosen direction. The photon generator is an n^+-p^+ doped-silicon diode. When biased in reverse just before avalanche, the additional electrons carried by the SAW will tip the balance and recombination should occur.

2.3 VECTOR NETWORK ANALYSIS

The IDT delay-lines were analyzed in a probe station with RF probes from *Picoprobe* connected to an *Agilent PNA-X N5244A* vector network analyser with a time domain feature. Figure 2.3 shows the scattering parameters of an ACT sample with double-finger IDT delay-lines for four wavelengths. The leftmost figure is an overview of the reflection parameter S_{11} . Well defined dips of the excited SAW resonances are visible, with three SAW modes per wavelength.

Figure 2.2: Optical images of different ACT devices with SEM close-up of active ACT areas. a) optical image of device with electrostatic constriction (quantum point contact), a)i) charge source, a)ii) charge detector, b) optical image of ACT active region in QPC device, c) SEM image of nanowire lead gates for injection of electrons into the SAW path, d) quantum point contact, e) optical image of electrostatic switch, and f) close-up of ACT area. Solid blue arrows indicate the path of SAWs from the IDT. In the optical images, light (grey) areas are metal and other areas the plain substrate. Square and dagger shapes are doped areas in the silicon with Ohmic contacts denoted by Ω . In SEM images the ZnO multilayer is visible with its characteristic grain structure. Most striking are the dark voids within the film, indicating missing grains which were most likely dislodged during the fabrication steps.

Figure 2.3: Vector network analysis of finalized and functional ACT sample. Outer left: an overview of the SAW resonances of the NIL IDTs. Right three: A close up on the resonances of $\lambda = 800$ nm. While the dips in the reflection means that SAW are being excited, the flat transmission indicates that propagation is very low. A small feature may be visible for S_{21} for R2.

The right-hand side of Figure 2.3 shows a closer look at the scattering parameters of the fundamental Rayleigh SAW mode R1, and following it, the higher-order Rayleigh modes labeled R2, and R3 for $\lambda = 800$ nm. The reflection dip in S_{11} is on the order of $\sim 0.25 - 0.5$ dB from a baseline of -3 dB, which means that only $\sim 5\%$ of the input power $P_{\text{in}} = 0$ dBm is being transferred from electrical RF to mechanical SAWs. Additionally, the transmission parameter S_{21} shows very little signal for the first two modes and a wide resonance for mode R3. The 800 nm wavelength device was chosen for acousto-electronic experiments, as it had the best transmission characteristics of the available devices.

2.4 OPTO-ACOUSTO-ELECTRONIC CHARACTERIZATION

The benchmark photon detection device is used to validate the functionality of the fabricated IDTs, the deposited piezoelectric thin-film material, and also of the doped silicon structures. The following experiments were carried out at the group of P.V. Santos at the Paul-Drude-Institut für Festkörperelektronik, Berlin.

Figure 2.4: Optical and acoustic check on a $\lambda = 800$ nm photon detection device at room temperature. Left: IV Response of the p-i-n diode with and without RF power on the IDT ($f_{RF} = f_{R2} = 5.97$ GHz). Right: A frequency sweep around mode R2, with the p-i-n diode in reverse bias. The light lines indicate where the SAW resonance is in the frequency space.

2.4.1 Experimental setup and characterization at 300 K

Figure 2.4a shows the I - V characteristics of the p-i-n diode in response to RF power on the IDT and laser-generated excitons at room temperature. The SAWs are generated using a *Rhode & Schwartz SMP02* RF generator with an RF amplifier *ZVA 1835+* attached to the output and the p-i-n diode IV response is measured with a *Keithley 2602 sourcemeter*. While the laser is switched off, and focusing on the diode in reverse bias ($V_{pn} < 0$), the negative current I_{pn} increases as the RF power is switched on ($f_{RF} = f_{R2} = 5.97$ GHz). This increase may indicate the presence of acousto-electric transport of free charges thermally excited at room temperature. To examine this effect we bias the diode in reverse ($V_{pn} = -2$ V) and sweep the frequency of the RF generator close to the R2 resonance of the IDT with the laser turned off and then on at a small power $P_{laser} = 20$ μ W (Fig. 2.4b).

We use a pulsed diode laser (*PDL 800-B*) with a wavelength of $\lambda_{laser} = 635$ nm to generate charge carriers for the ACT effect. The laser is positioned approximately 50 μ m away from the IDT (see Fig. 2.1b) and is focused to a spot size of ~ 6 μ m by a *Mituyoto F570L* microscope objective lens. The laser power P_{laser} is measured with a *PM100D laser powermeter*. The background I_{pn} does not change appreciably, neither with more RF power, nor with additional carriers being generated by the laser. Thus, the effect is both RF and laser independent at room temperature.

Figure 2.5: VNA of $\lambda = 800$ nm photon detection device at $T = 10$ K. Left: mode R1, Right: mode R2. Both modes are shown with time-gating for the transmission S_{21} and are detected at a very low power. Mode R3 was not seen.

2.4.2 Characterization at 10 K

Lowering the temperature decreases phonon scattering of the SAW and may result in better transmission and current characteristics. The sample is cooled down in a high-vacuum probe station from *Süss MicroTec* with liquid helium and a base temperature of 10 K. Figure 2.5 shows the scattering parameters of the first two SAW modes of $\lambda = 800$ nm, measured with an *Anritsu MS46522B* network analyzer. The reflection dip in S_{11} is comparable to room temperature ($\sim 0.25 - 0.5$ dB) and the transmission is also very low, even when time-gating is used (peak in $P_{21} \approx -100$ dB for R1 and $P_{21} \approx -80$ dB for R2). Thus, while the transmission of the traveling SAW is detected, the power and the amplitude may be too low for measurable ACT. The frequency of the resonance is expected to rise at lower temperatures, given the increase in material density and acoustic velocity. For mode R1, the temperature frequency change is not appreciable and for R2 the change is less than 50 MHz. This corresponds well to a SiO_2/ZnO multilayer structure, as the materials have an opposing temperature coefficient of frequency (TCF). However, this material system has not been optimized for TCF for either mode.

In Figure 2.6 we show the dependence of the p-i-n diode dark current I_{pn} for a wide frequency sweep of the RF power. The sample is at 10 K, with both the laser and RF power at maximum, $P_{\text{laser}} = 210 \mu\text{W}$ and $P_{\text{SAW}} = +26$ dBm, respectively. The expected frequencies of the SAW modes are highlighted with vertical lines. The resulting current fluctuates wildly over several tens of nA and has no clear increase or feature corresponding to ACT at the established SAW resonance frequencies. The large noise in the current comes from RF electromagnetic (EM) interference generated by the IDT which acts as an antenna.

Figure 2.6: RF frequency dependence of p-i-n diode current I_{pn} for a $\lambda = 800$ nm photon detection device at $T = 10$ K. Various current fluctuations are seen for many frequencies, most likely due to the EM output of the IDT. The expected frequency position of the SAW resonances is highlighted by a line for each mode. No discernible SAW ACT effect is seen.

2.4.3 RF and laser triggering

One way to minimize such EM interference, is by timing the generation of both SAWs and laser pulses to ensure that no RF power is on the IDT as the SAW reaches the p-i-n diode. As the EM velocity is much greater than the acoustic velocity, the acoustic delay of the SAW from the IDT to the p-i-n junction can be used as the RF power cut-off time. Therefore, the measured current signal from the diode will not have an EM component.

Figure 2.7 gives an overview of timed generation with a block diagram (left) and the model of operation (right), similar to a pulse scheme used in [34]. As seen in Fig. 2.7a, the RF generator (*R&S SMP02*) is set to send a low-frequency trigger signal with an RF pulse (with power P_{RF}) of set duration, repetition rate, and delay. The trigger signal also initiates a function generator (*Tektronix AFG3101*), which sends a pulse burst to the laser diode resulting in laser power P_{laser} . The delays are adjusted with the help of an oscilloscope (*Agilent technologies MSO 6104A*), such that the laser is activated just after the SAW.

Figure 2.7b illustrates a triggering model in practice. The bottom part gives the approximate dimensions of the photon detector main components; the IDT with a length of $l_{IDT} = 350$ μm , the position of the laser spot from the IDT $d_s = 90$ μm , and distance of the p-i-n diode from the IDT $d_{pin} = 275$ μm .

Figure 2.7: Block diagram and expected output of a trigger setup for the RF and laser power. Left: Block diagram of used instruments and their connections. Right: Expected output of trigger setup. A triggering pulse is sent out of the RF generator, which switches the laser and RF power on after a set delay and for a set duration. The timing can be made such that only when the SAW is traveling out of the IDT, the laser is on. This reduces the EM output noise of the IDT.

The trigger functions in the following way: at time $t = 0$ ns (Fig. 2.7b(i)), the RF pulse P_{RF} is triggered and a SAW is generated at the IDT (marked by a blue rectangle). Approximately fifteen nanoseconds later (ii), the SAW reaches the laser spot and the laser power is triggered P_{laser} (red). The calculation for this delay ($t_{\text{delay}} = d_s/v_{\text{SAW}}$) depends on the SAW velocity, which for the fundamental mode R1 is $v \approx 3,100 \text{ m s}^{-1}$ (for frequency $f_{\text{R1}} = 3.9 \text{ GHz}$ and device wavelength $\lambda = 800 \text{ nm}$). The SAW, now dragging excitons, reaches the p-i-n diode at $t \approx 100 \text{ ns}$ and the RF power is switched off (iii). The SAW generated at the other end of the IDT from the p-i-n diode still has to travel through the whole IDT length and does so around $t \approx 200 \text{ ns}$ (iv). The laser can be switched off after $t \approx 215 \text{ ns}$ as the tail of the SAW reaches the laser spot (v). The SAW tail exits the p-i-n diode at $t \approx 300 \text{ ns}$, ending the trigger cycle (vi).

We used the following parameters for the trigger setup. The trigger frequency was set to $f_{\text{LF-t}} = 1 \text{ kHz}$ (100 kHz), the SAW pulse period $p_{\text{SAW}} = 1 \mu\text{s}$, and the SAW pulse width $t_{\text{SAW}} = 200 \text{ ns}$ ($5 \mu\text{s}$). The laser pulse was set to the maximum $f_{\text{laser}} = 40 \text{ MHz}$ and a duration of 14 (200) cycles with a delay to the SAW pulse of $t_{\text{delay}} \approx 25 \text{ ns}$. The output laser power measured by

Figure 2.8: Triggered-RF frequency dependence of p-i-n diode current I_{pn} for a $\lambda = 800$ nm photon detection device at $T = 10$ K. The various current fluctuations in Fig. 2.6 are suppressed. The expected frequency position of SAW mode R1 is highlighted by a line. Unfortunately, no discernible SAW ACT effect is seen.

the laser powermeter with such a trigger setup is $P_{\text{laser}} = 10 \mu\text{W}$ ($63 \mu\text{W}$). The values in parenthesis were used to maximize laser power output and SAW duration in later *IV* measurement attempts.

The effect of the triggering setup on the p-i-n diode current I_{pn} is shown in Figure 2.8. At first glance, the frequency dependent current is much less noisy than in Figure 2.6 and thus, the EM interference is suppressed. However, there is no sign of any acousto-electronic driven increase of the dark current at the expected resonance frequency. Small fluctuations in the current are attributed to imperfect measurement conditions and noise.

While the triggering setup does help suppress contribution from the EM background generated by the IDT, no ACT was detected even with higher laser and RF power settings. This is due to the very poor propagation of traveling SAWs in the sputtered multilayer thin-films as seen in Fig. 2.4. The material origin of the SAW loss will be analyzed in the following Chapter (Chapter 3).

2.5 DISCUSSION AND CONCLUSION

We fabricated acousto-electronic transport devices on silicon using a combination of optical, nano-imprint, and electron-beam lithographic methods. We found damage to the active piezoelectric thin-film after the device fabrication

with SEM imaging (Fig. 2.2). The network analysis of the IDT delay-lines for SAW generation showed low power conversion and poor transmission of propagating SAWs.

Cooling the sample down to $T = 10\text{ K}$ improved SAW transmission only marginally, while confirming temperature-driven frequency change to be small due the complimentary ZnO/SiO₂ material TCF parameters. During acousto-transport experiments, an overwhelming contribution to the dark current was in the form of electromagnetic interference. A triggering and timing setup suppressed the EM coupling of the IDT and diode, however, no detectable ACT effect was seen, which is attributed to the poor thin-film material quality for traveling SAWs.

Several improvements to IDT and ACT device design and fabrication are needed. First, optimization of piezoelectric thin-films at low thicknesses is a necessity for high-frequency acousto-electronic transport. In addition, nano-imprint lithography has many fabrication and substrate surface quality constraints and thus, better surface layers are compulsory. Further, since fabrication is damaging to the sputtered piezoelectric thin-films, an alternate process in which the thin-films are deposited in the last steps of processing is desirable. Alternatively, piezoelectric thin-films such as AlN or bonding of single-crystal materials on top of functionalized silicon may offer more attractive avenues of silicon acousto-electronics implementation.

In the following chapters, we explore the thin-film material origin of poor SAW transmission and we offer an in-depth look at the efficiency of IDT generation of the high-frequency SAWs via impedance matching with numerical models.

DEFECT ORIGIN OF ACOUSTIC PROPAGATION LOSSES IN ZnO THIN-FILMS ON SILICON

3.1 INTRODUCTION AND DEVICE STRUCTURE

Silicon acousto-electronic devices need an additional piezoelectric layer to excite surface acoustic waves and successfully operate. Thin-film piezoelectric materials are widely used in industry for RF filters in so called 'slow on fast' configuration to access higher frequencies by SAW penetration into the acoustically faster silicon substrate. However, not all materials are compatible with integration, nor capable of growth on silicon substrates. Even more, relatively thick films ($> 1 \mu\text{m}$), desirable for their better poly-crystalline properties, prohibit SAWs with smaller wavelengths of penetrating into the substrate.

Here, we use a SiO_2 (20 nm)/ZnO (100 nm)/ SiO_2 (100 nm) multilayer on silicon as the functional piezoelectric layer. The thick bottom SiO_2 serves two roles; as an insulator, separating the ZnO and Si underneath, and as a waveguide, for the excitation of higher-order, high-frequency SAWs.

For material comparison, three different deposition techniques are used to grow a 100 nm ZnO layer. The resulting thin-film multilayer is examined by material characterization techniques and electrically via delay-lines for suitability in silicon acousto-electronic transport (ACT) experiments.

3.1.1 Fabrication

Fabrication starts first with an intrinsic silicon 100 mm substrate (resistivity $\rho > 10 \text{ k}\Omega \text{ cm}^{-1}$), which is thermally oxidized at $1,050^\circ\text{C}$ in a dry oxidation oven to form 100 nm of thermal oxide. Secondly, the piezoelectric material ZnO is deposited using three different methods from three different sources; sputtering at Paul-Drude-Institut für Festkörperelektronik Berlin, pulsed-laser deposition (PLD) at Solmates and sol-gel at the University of Twente. Thirdly, a capping layer of 20 nm SiO_2 is sputtered onto the ZnO. And lastly, delay-lines are fabricated using nano-imprint lithography.

3.1.2 ZnO deposition

The first two methods of ZnO deposition are well known for their application in thin-film growth. Radio-frequency magnetron sputtering of piezoelectric thin-films is used in industry for RF filters and MEMS. Pulsed-laser deposition is interesting for epitaxial growth of complex oxides. In this work, the deposition process is similar to the one used in Ref. [22] for sputtering and the one used in Ref. [35] for PLD.

As a third method of ZnO deposition, we chose sol-gel due to its desirable crystalline properties, ready availability, and compatibility with cleanroom processing and nano-imprint lithography. In our work, we based the sol-gel synthesis on the recipe of Wang et al., 2007 [36], after a review of literature focused on sol-gel ZnO thin-film with (002) poly-crystalline alignment (see also Ref. [37]).

First, we start with the preparation of a Monoethanolamine (MEA) solution in ethanol. MEA, which is both a complexing and interface agent, is added to ethanol to a concentration of 1.2 mol l^{-1} and magnetically stirred at room temperature for 10 min. Next, a zinc source is used, in this case zinc acetate dihydrate (ZAD), to achieve a molar ratio of $[\text{Zn}^{2+}]:[\text{MEA}] = 2:3$. The solution is then magnetically stirred at 60°C for 2 hours with reflux. Afterwards, the resultant sol-gel is aged in a refrigerated environment for 24 hours. Before use, the sol-gel is transferred to a new holder through a $0.2 \mu\text{m}$ filter. The sol-gel looks clear, with no color and no visible precipitates.

We spin-coat the sol-gel in a cleanroom environment to preclude any particles from contaminating the resulting thin-films. We apply a set volume per layer of the sol-gel to an oxidized Si wafer while it is already spinning at 3,000 rpm for 10 s. Then the spin speed is increased to 4,000 rpm for an additional 30 s. After the spin-coating, the wafer is baked at 250°C for 10 min to evaporate the ethanol and MEA solution. We repeat this process three times, with one layer averaging a thickness of 40 nm, for a total ZnO layer thickness close to 120 nm. Finally, the wafer is thermally annealed in an oven with an atmospheric gas mixture at 500°C for at least 2 hours.

3.2 ZnO THIN-FILM CHARACTERIZATION

We compare the deposited $\text{SiO}_2/\text{ZnO}/\text{SiO}_2$ multilayers by surface and material characterization techniques, namely, scanning electron microscopy (SEM), X-ray diffraction (XRD), and atomic force microscopy (AFM). To determine the S-parameters of the delay-lines, a vector network analysis of the fabricated delay-lines is carried out to find and characterize SAW resonances.

Figure 3.1: Scanning electron microscope images of ZnO thin-films with NIL IDTs. a) sputtering, b) PLD, c) sol-gel, and d) sol-gel on a plain sample with better contrast. Visible are pinholes in the sputtered and PLD thin-films and the sol-gel film is quite porous.

3.2.1 Scanning Electron Microscopy

The finished samples with NIL delay-lines are first imaged with SEM to verify the IDT structure. While the IDTs are without defects, immediately evident are discontinuities and voids in the ZnO multilayers as seen in Figure 3.1. The presence of pinholes and gaps in the films in the sputtered and PLD films, in Figures 3.1a and 3.1b, increase SAW diffraction and are a great source of loss. Furthermore, while pinholes are found next to the IDTs, they are also present underneath them. These pinholes, however, are smaller and less common, which may suggest a fabrication-related component in their origin and nature.

In-principle, the thin-films is protected by the capping layer of 20 nm SiO_2 . However, during nano-imprint fabrication certain steps may lead to film degradation and we shall look more closely at three: ultrasonic cleaning, lift off, and reactive ion etching (RIE).

Before NIL can proceed, the substrate with the piezoelectric multilayer has to be cleaned first in an acetone, then an 2-isopropanol, and finally a DI wafer ultrasonic bath. Here, particles within the film, from before or during thin-film deposition, may be dislodged. The substrates are checked under an optical microscope before further NIL processing for particles and pinholes. PLD films had large particles visible and they were clearly within the thin-film. Sol-gel films had many pinholes, visible only as small, circular discolorations of the film. Only sputtered films looked uniform and without large particles. During lift-off the sample is also in a DI water ultrasonic bath and after this last step the pinholes usually become more evident. DI water is quite aggressive to certain materials and ZnO may be chemically dissolved and mechanically attacked.

Dry reactive ion etching is another potential source of film damage. During this step, the NIL resist is etched to transfer the IDT pattern down to the substrate. The substrate is cooled during this step and this can lead to film degradation. However, this would be evident in both optical and electron microscopy images as larger fractures and fissures.

A more likely scenario is the following: since the film has particles, which may be dust or from the deposition target material (i.e.: PLD), the 20 nm SiO₂ capping layer cannot form a perfectly sealed film around them. This in turn makes them vulnerable to mechanical detachment, especially after a temperature cycle as the film contracts. Thus, the initial cleaning is largely safe, even the spin-coating and baking of NIL layers, but after the RIE step, the particle can be susceptible to mechanical vibration in an ultrasonic bath. The particles detach and the rest of the surrounding film is sensitive to mechanical and chemical erosion, as it could not integrate well during growth.

The sol-gel film appears more uniform in Fig. 3.1c, although a better SEM image (Fig. 3.1d) away from the IDTs reveals that the density of defects is even higher than that for sputtered or PLD films. Additionally, the film is very porous, which is detrimental for SAW generation and propagation.

The films are then checked with X-ray diffraction to determine their crystallinity, as described in the following section.

3.2.2 X-ray diffraction

X-ray diffraction was carried out on 1.5×1.5 mm pieces taken from near the center of SiO₂/ZnO/SiO₂/Si multilayer 100 mm substrate by a *PANalytical X'pert*. Two measurements were performed on each sample piece, a θ - 2θ scan around the characteristic (002) Wurtzite ZnO peak and an omega scan centered on the detected peaks.

The XRD analysis results are shown in Fig. 3.2, in which all three polycrystalline ZnO films have a peak in intensity around 34.4° corresponding to

Figure 3.2: X-ray diffraction measurements of ZnO thin-films from three origins; sputtering (PDI Berlin), PLD (Solmates) and sol-gel (Univeristy of Twente). All three ZnO polycrystalline films exhibit (002) Wurtzite structure perpendicular to the surface. Both sputtering and PLD have a clear higher fraction of crystallites in this orientation. The sol-gel film also shows additional side peaks, corresponding to the (010) and (011) orientations, indicating a partial mix of growth directions. The inset, an omega scan around the (002) peaks for all three films, shows that only sputtered and PLD films have any uniformity of in-plane orientation and texture. The grey dashed line indicates the position of the reference ZnO (002) peak from Ref. [38].

the out-of-plane (002) ZnO crystal orientation. The grey dashed line indicates the position of the reference ZnO (002) peak from Ref. [38]. All three films show good (002) orientation, however the PLD film has a deviation from the reference and may be strained. The sputtered and PLD films have clearly a higher fraction of crystallites in the (002) orientation due to their peak height. Furthermore, the sol-gel shows additional peaks at 31.8° and 36.4° , corresponding to the (010) and (011) orientations, respectively. The inset, an omega scan around the (002) peaks for all three films, shows that only sputtered and PLD films have some uniformity of the in-plane orientation and texture. The broad omega peaks indicate that individual grains are relatively poorly oriented in the in-plane and show mosaicity. Additionally, structural and height non-uniformities maybe prevalent which agrees with the SEM images in Section 3.2.1. Using the Scherrer formula, the mean grain size $\bar{D}$ is estimated to be around 25 nm for all three films, shown in Table 3.1 [39]. However, this method of estimation is known for large errors. For a more

Table 3.1: XRD extracted parameters of ZnO thin-films. The position of the peak in 2θ , its FWHM and the grain size $\bar{D}$ extracted with the Scherrer equation [39]

deposition	2θ [°]	FWHM [°]	$\bar{D}$ [nm]
sputtering	34.41	0.3223	25.79
PLD	34.5	0.3208	25.91
sol-gel	34.41	0.337	24.66

detailed examination of the thin-film surfaces, AFM was chosen as the next step.

3.2.3 Atomic Force Microscopy

As a final analysis of the film material quality, an AFM scan was carried out using a *Bruker AFM Icon*. The area of scan is $2 \times 2 \mu\text{m}$ and situated close to the IDTs, as seen in the SEM images (Fig. 3.1). The scanned AFM micrographs for all three films were processed with the open-source software Gwyddion.

First, the micrographs are flattened using a polynomial background subtraction. Next, they are amended to exclude erroneous data, such as off-scale spots most likely from contaminants. The resulting micrographs can be seen in Figure 3.3. And finally, a grain analysis is used by using an adjustable grain finding procedure that estimated the size and positions of grains based on the height data within the micrograph. The three resulting quantitative analyses contribute to an overall picture of the texture of the film at the micrometer scale and are summarized in Table 3.2.

In considering the micrographs, one should notice the maximum of the height scale bar next to the three figures. It is readily apparent that there is a scale to the height variations between samples, from lowest for the sputtered material, to highest for the sol-gel film. This can also be seen in the mean grain height statistic in Table 3.2.

The topology is quite different for the three films and goes from smoothest for sputtering to rougher for sol-gel, with PLD in the middle of the two. The RMS roughness goes from $S_q < 1 \text{ nm}$ to $S_q \approx 6 \text{ nm}$, for sputtering and sol-gel respectively. The AFM micrograph of the sputtered thin-film is of lower quality than the other two, but the expected roughness is not expected to be more than the roughness for PLD, which is $S_q \approx 3 \text{ nm}$. The estimated mean size of grains, $\bar{D}$, for the three films is highest for the sputtered and lowest for the PLD. This is different from the estimates obtained from the XRD analysis using the Scherrer formula. And finally, the height distribution for the grains in the scanned area shows the highest variation for sol-gel ($\approx 34 \text{ nm}$) and the lowest for sputtering ($\approx 9 \text{ nm}$).

Figure 3.3: Atomic force microscope micrographs of ZnO thin-films. a) sputtering, b) PLD, c) sol-gel, and d) a pinhole (sputtering). The scan areas are $2 \times 2 \mu\text{m}$. The height variations of each surface are visible, where sputtered material appears to be the least rough of the three. Detailed statistics of each film can be seen in Table 3.2. The presence of a pinhole alters the local roughness of the film significantly.

An additional AFM scan of a pinhole feature in a sputtered ZnO/Si piezoelectric multilayer is shown in Figure 3.3d. One can see a textured film surrounding a circular feature of decreasing height with a central cavity. The RMS roughness is approximately $S_q \approx 1.9 \text{ nm}$ without the valley feature, but climbs to $S_q \approx 9 \text{ nm}$ for the whole micrograph. The active sample area of our delay-lines is approximately $50 \times 1,000 \mu\text{m}$, while the pinholes are on the order of $1 \times 1 \mu\text{m}$, hence, the resulting roughness may not have a drastic effect on SAW performance. However, there may be a limit to the pinhole density, beyond which SAW propagation is diminished to undetectable levels.

Delay-line performance as compared to the determined material properties in this section can be assessed when combined with electronic measurements, such as vector network analysis of SAWs excited by the fabricated IDTs.

Table 3.2: Atomic force microscope micrograph statistics of ZnO thin-films. A statistical analysis was performed on the AFM images in Fig. 3.3. An intricate interplay of factors contributes to the functionality of the thin-film. The grain size is different than that estimated by the XRD.

deposition technique	RMS roughness [nm]	mean grain size $\bar{D}$ [nm]	mean grain height [nm]
sputtering	< 1	37.9 ± 5.7	8.9 ± 0.6
PLD	2.9	18.6 ± 2.7	12.7 ± 2.3
sol-gel	6.4	30.7 ± 6.2	33.5 ± 3.5

3.3 ELECTRICAL CHARACTERISATION

In this section, we analyze the piezoelectric properties of $\text{SiO}_2/\text{ZnO}/\text{SiO}_2/\text{Si}$ multilayer thin-films with a focus on surface acoustic waves and their propagation with fabricated NIL IDT delay-lines. There are four wavelengths investigated: $\lambda = 1,000 \text{ nm}$, 800 nm , 640 nm , and 520 nm , corresponding to double-finger IDT feature sizes 125 nm , 100 nm , 80 nm , 65 nm , respectively. At the end of this section we also examine the change in SAW propagation when the SiO_2/ZnO multilayer is removed in-between the IDTs.

3.3.1 Vector network analysis (VNA)

The fabricated IDTs are contacted in a probe station using G-S RF probes up to 40 GHz from *Picoprobe* connected to a *R&S ZVB20 4-port Network Analyzer* or *Agilent PNA-X N5244A* vector network analyzer with time domain. The network analyzer was calibrated before measurement using a calibration substrate in the case of the *ZVB20* and using an electronic calibration module in the case of the *PNA-X*.

The IDTs were first made of a Cr/Al ($5/35 \text{ nm}$) stack, which discontinued to function after several days, most likely due to oxidation. As an alternative for later samples, a $\text{Ti}/\text{Al}/\text{Ti}$ ($5/20/10 \text{ nm}$) or Cr/Au ($5/35 \text{ nm}$) stack was used and these continued to function reasonably for further measurements.

Both the sputtered film and PLD film were analysed using the *PNA-X* VNA. The scattering parameter S_{11} (reflection) for IDTs of various wavelengths on the sputtered and PLD films in Figure 3.4 shows many resonance dips for each wavelength. When present, these correspond to the Rayleigh, Sezawa and third SAW mode, starting respectively from lowest frequency dip of each trace [28].

The measured SAW resonances start at $f_{\text{SAW}} = 3.6 \text{ GHz}$ for double-finger (DF) $\lambda = 1,000 \text{ nm}$ IDTs (fundamental SAW - Rayleigh mode - R1) and go up

Figure 3.4: Vector network analysis of NIL IDTs on a SiO_2 (20 nm)/ZnO (100 nm)/ SiO_2 (100 nm)/Si multilayer. Reflection scattering parameters S_{11} are shown for both, a) sputtered and b) PLD ZnO. The excitation of SAWs results in a dip in the reflection as RF voltage is converted via the converse piezoelectric effect to mechanical deformation within the ZnO layer at resonant frequencies corresponding to $f_{\text{SAW}} = v_{\text{SAW}}/\lambda_{\text{SAW}}$. Traces in both graphs were offset for better visibility. Sol-gel ZnO did not excite any SAWs. An overview of the SAW frequencies and resulting characteristics can be seen in Table A.2.

to $f_{\text{SAW}} = 12.7 \text{ GHz}$ for single-finger (SF) $\lambda = 260 \text{ nm}$ IDTs (higher-order SAW - Sezawa mode - R2). The corresponding SAW velocities are approximately $v_{\text{SAW}} = \lambda_{\text{SAW}} \cdot f_{\text{SAW}} = 3.6 \times 10^3 \text{ m s}^{-1}$ and $3.3 \times 10^3 \text{ m s}^{-1}$, respectively. An overview of the measured SAW frequencies, calculated velocities and the resulting effective electromechanical coupling constants can be seen in Figure 3.5. A table with all the values is in Appendix A.1. In the following sections we shall discuss the interplay of the ZnO multilayer, IDT wavelengths and electrodes on the resulting SAW characteristics.

As one would expect, the frequencies of the excited SAWs are generally increasing with decreasing wavelength. The higher-order SAW modes have correspondingly higher frequencies. This is characteristic of piezoelectric thin-film multilayers on acoustically fast substrates. In this case, the SAW velocity in ZnO is close to the transverse bulk acoustic velocity $v_{\text{TZnO}} = 2.73 \times 10^3 \text{ m s}^{-1}$, whereas, the velocity in the surrounding SiO_2 and underlying substrate is much higher, $v_{\text{TSiO}_2} = 3.6 \times 10^3 \text{ m s}^{-1}$ and $v_{\text{TSi}} = 5.85 \times 10^3 \text{ m s}^{-1}$ respectively [7, 28]. This creates a focusing of the SAW electric field in the ZnO and thus, the strain field as well, similar to waveguiding, which evokes more complexity of the SAW penetration of the substrate [40]. Higher-order SAW modes have been studied before for their inherent high frequencies [13]. For the purpose of this research, we take advantage of their higher phase

Figure 3.5: Analysis of VNA measurements of NIL IDT delay-lines on a SiO_2 (20 nm)/ZnO (100 nm)/ SiO_2 (100 nm)/Si multilayer. Top segment shows measured frequency, middle: calculated velocity, and bottom: calculated experimental electromechanical coupling coefficient K_{exp}^2 . While the frequency response of the IDTs increases with smaller wavelength as expected, the velocity decreases slightly. This is due to a smaller fraction of the SAW penetrating into the substrate. K_{exp}^2 is higher for smaller wavelengths due to the interplay of ZnO/ SiO_2 layer thicknesses.

velocities, thus higher frequencies, and their more structured electric field penetration into the substrate, where local maxima are situated more closer to the targeted acousto-electric transport medium, i.e. the silicon substrate. A more detailed examination of the higher modes with numerical simulation is shown in Chapter 5.

Further, one can notice an interesting detail typical of sub-micron wavelength IDTs between the two figures. The Rayleigh resonance of a smaller wavelength IDT $\lambda = 500$ nm has a smaller frequency than the larger wavelength $\lambda = 520$ nm in Figure 3.5. We shall discuss three possible sources of this discrepancy.

The first source, is that the nominal film thickness is an estimation from the suppliers and maybe be slightly thicker or thinner than expected. The second, is related to the first; the penetration of the SAW into the substrate plays an important role. The fraction of the SAW in a fast or slow acoustic material determines the overall SAW velocity. The parameter related to this is the thickness-wavelength ratio h_{ZnO}/λ . For the wavelength $\lambda = 1,000$ nm

it is close to $h_{\text{ZnO}}/\lambda = 0.1$ and thus, more of the wave penetrates into the substrate. For the smallest wavelength $\lambda = 260$ nm, $h_{\text{ZnO}}/\lambda = 0.38$ and taking into account the whole ZnO multilayer thickness $h = 220$ nm, leaves less than 40 nm of the SAW is within the silicon substrate. The velocity segment of Figure 3.5 shows a general decline in velocity with smaller wavelength, indicating less SAW penetration into the acoustically faster substrate.

Thirdly, the electrode material is different, specifically, the sputtered ZnO has Cr/Al DF IDTs and the PLD ZnO has Cr/Au SF IDTs. Gold is much heavier than aluminum and for low wavelengths the electrode thickness h_{el} is more critical as it influences the SAW frequency via its weight. This effect can be described by the electrode thickness and wavelength ratio h_{el}/λ . In industry, for SAW filters, the ratio is kept very low, ca. $h_{\text{el}}/\lambda < 0.01$. In our devices, we start at $h_{\text{el}}/\lambda = 0.04$ for $\lambda = 1,000$ nm and exceed $h_{\text{el}}/\lambda = 0.1$ for the smallest wavelength $\lambda = 260$ nm. The IDT and material characteristics for wavelengths can be seen in Table A.2. The influence of electrode and material thickness on SAW frequency and SAW-substrate coupling is shown in Chapter 5.

The conversion efficiency of the electric impulses on IDT to mechanical deformation in the piezoelectric material is described via the effective electromechanical coefficient K_{exp}^2 . It is calculated from the impedance characteristics around SAW resonance of the scattering parameter S_{11} [10] and is shown in the bottom section of Figure 3.5. Double-finger IDTs ($\lambda \geq 520$ nm) show a similar K_{exp}^2 for all SAW modes, whereas for single-finger IDTs ($\lambda \leq 500$ nm) the higher modes have a higher coupling efficiency. The interplay of layer thickness, wavelength, IDT design and impedance matching to the substrate is shown in a more detailed examination of impedance matching is given in Chapter 5.

Unfortunately, the transmission parameter S_{21} for both ZnO multilayers generally gave very small or no signal. However, we now examine measurements from one working sputtered ZnO sample in Figures 3.6 and 3.7.

The measured transmission of a $\lambda = 1,000$ nm delay-line is in Figure 3.6. In the top figure (Fig. 3.6a), are three dips immediately visible in the reflection with three corresponding features in the transmission.

A closer look at the first two SAW modes, R1 (Rayleigh) and R2 (Sezawa), is shown in the lower figure (Fig. 3.6b), both with and without time-gating. Time-gating the transmission signal S_{21} is analogous to narrow bandwidth frequency filtering, just in the time domain. We applied time-gating with time windows ~ 100 ns – 400 ns and filtered the SAW signals from the microwave electromagnetic background. Only the R1 mode is visible without time-gating and is quite low above the noise level, about 5 dB. It shows a structure characteristic of a resonator, with many lobes and oscillations making up the peak. The reason can be two-fold: one, the resulting delay-lines have in fact standing waves in-between them, and two, the IDT itself is very reflective and has many

Figure 3.6: Vector network analysis of NIL $\lambda = 1,000$ nm IDTs on a SiO_2 (20 nm)/ZnO (100 nm)/ SiO_2 (100 nm)/i-Si multilayer. a) A trace capturing all three resonances of the delay-line. The two sharp dips, R1 and R2, in S_{11} are the Rayleigh and Sezawa modes, respectively. The third is more broad in reflection and has more features in the transmission. Only R1 is seen and has any structure without time-gating the transmission. Both transmission peaks are still very low in the sub- 80 dB range. Overall, poor transmission of the SAWs in these delay-lines.

Figure 3.7: Vector network analysis of NIL $\lambda = 800$ nm IDTs on a SiO_2 (20 nm)/ZnO (100 nm)/ SiO_2 (100 nm)/i-Si multilayer. Left: A VNA trace capturing two resonances of the delay-line. The two sharp dips, R1 and R2, in S_{11} are the Rayleigh and Sezawa modes, respectively. There are no corresponding features in the transmission. Middle: A close up of the Rayleigh mode. The transmission is seen only with time-gating and is very low in power, below 100 dB. Right: A close up of the Sezawa mode. No appreciable transmission is seen even with time gating. Overall, very poor transmission of the SAWs in these delay-lines.

internal reflections of the SAWs both arriving at and originating from it. The R2 mode is not directly visible without time-gating and appears only as a very small peak. Both transmission peaks are still very low in the sub- 80 dB range. The third peak is broader in both the reflection and the transmission, possibly a spurious acoustic wave such as a surface skimming bulk acoustic wave.

A closer look at the transmission of the $\lambda = 800$ nm delay-line is shown in Figure 3.7. Here, an even lower transmission signal is seen, as R1 (middle figure) is visible only with a time-gate and R2 (right figure) is not visible at all.

Finally, sol-gel ZnO did not excite any SAWs. This may be primarily due to the density of the film, notwithstanding any crystalline defects of the polycrystalline film. Two approaches were tried to increase the viability of the ZnO sol-gel thin-film for acoustic application. A thicker film of up to 7 spin-coating rounds was created, resulting in an approximately 300 nm thick film, and complimentary, a longer 10 hour thermal annealing step. Neither configuration resulted in functional ZnO thin-films for SAWs.

Clearly, for these ZnO/Si material multilayers, with the discussed composition and properties, there is a strong attenuation for higher frequencies.

However, not everything can be laid at the feet of the material. The IDTs themselves are quite reflective and thus, the impedance mismatch of the RF to the IDT must be taken into account. Likewise, the acoustic coupling of the SAWs from the IDT region into the propagation region is critical. If the SAW reflection off an IDT edge is high, most of the SAW will not travel out of the IDT. Impedance mismatch and IDT reflectivity will be discussed in Chapter 5.

3.4 WET ETCHING OF ZnO

The next question naturally becomes: can we have our cake and eat it too? That is to say can we use the defective $\text{SiO}_2/\text{ZnO}/\text{SiO}_2$ to generate SAWs, but alter it to increase propagation? One of the ways this can be explored is to etch away the multilayer in-between the regions of the IDTs.

To determine the effect of the sputtered layers on traveling SAWs in a ZnO/Si multilayer, one can remove it between the transmitting and receiving IDTs and compare transmission scattering coefficient S_{21} before and after.

In order to remove the materials, wet chemical etching is chosen as the most direct and efficient option. First, the IDT contacts are covered with a thicker contact pad of ca. 100 nm of gold. Next, optical lithography is used to define the etch areas and protect the IDT and contact pad regions. The sample with developed resist is baked on a hotplate set to $T = 120^\circ\text{C}$ for 5 minutes for hardening.

The thin-film layer at the surface, the capping layer of 20 nm of SiO_2 is etched by a BHF dip of up to 10 s. Next, the ZnO layer is etched with (100 nm) a highly diluted HCl solution of 0.5 % for a further 10 to 20 s. The third layer on the silicon wafer is 100 nm of thermal SiO_2 and is left intact as this layer has a higher material quality. After each etch step, the sample is rinsed in a replenishing DI water bath for 5 min until the DI water resistance equals 10 M Ω . The samples are then checked under an optical microscope. The delay-line S-parameters are measured with a VNA R&S ZVB20 before and after etching and can be seen in Figure 3.8.

The left panel of Figure 3.8 shows the delay-line S-parameters before the etching. Small dips in the reflection S_{11} are present, characteristic for SAW resonances, with no sign of corresponding peaks in transmission S_{21} , which is similar to Fig. 3.4. A close-up of the deepest reflection dip around 5.55 GHz in the middle panel of Figure 3.8 shows a small response visible in the transmission, barely above the noise level.

After etching, the resulting S-parameter characterisation shows improvement in signal for both reflection and transmission in the right panel of Figure 3.8. Indeed, almost a doubling of the dip depth and peak height occurs with characteristic additional resonance lobes in the transmission.

Figure 3.8: Vector network analysis of NIL IDTs on a $\text{SiO}_2/\text{ZnO}/\text{SiO}_2/\text{Si}$ multilayer before and after wet etching. Left: A VNA showing both S_{11} and S_{21} of a SAW delay-line. Seen are characteristic dips in reflection, but no corresponding peaks in transmission. Middle: A close up around 5.5 GHz reveals a small rise in the transmission. Right: VNA after wet chemical etching of the SiO_2 capping and ZnO layer. Both reflection and transmission show some improvement.

The transmission signal improvement means better SAW propagation between IDTs, most likely due to the single-crystal silicon substrate. However, the overall signal strength still remains low, thus, one still needs to pay attention to the generation of SAWs and their coupling to the propagation region from the IDT. After etching, the IDT stands on an island of piezoelectric material. Generation of SAWs is still influenced by the material flaws discussed in Section 3.2.1 (e.g. Fig. 3.1), as are potential IDT impedance mismatches (which will be discussed in more detail in Chapter 5). For propagation, there is now a discontinuity of the surface at the edges of the IDTs equivalent to an additional reflection plane making the IDT island into a resonator by nature.

The coupling of the SAW from this resonator island to the propagation region seems to be reasonable, as can be seen in the right Fig. 3.8, however, perhaps not ideal. Further, the propagation region itself becomes a cavity since it lies between two IDT islands. The shift from propagating SAWs to resonating cavities may not suit acousto-electronic transport experiments as they rely heavily on the presence of traveling waves to drag electronic carriers from source to detecting regions. Even more, by removing the ZnO the SAW propagates only as a strain field in the remaining SiO_2/Si and not with the accompanying electric field when present in piezoelectric materials.

The acousto-electric effect is many times smaller for a purely moving strain field as for one with an electric field component, thus reducing the chance of detection even further.

3.5 DISCUSSION AND CONCLUSION

In this chapter we have fabricated and analyzed NIL IDT delay-lines on ZnO/SiO₂ multilayer on silicon. From the material side, our thorough analysis show numerous deficiencies such as large pinholes and contaminates, which contribute to large losses during SAW propagation. The textured polycrystalline thin-films showed best characteristics for the sputtered films, in both XRD and AFM. However, the SEM images reveal that the surface suffers from many cavities and defects.

From the electrical side, only the sputtered and PLD films are responsive to electrical excitation via NIL IDTs. Both films show they can generate SAWs, but propagation is an issue. The nature of the attenuation and overall low transmission amplitude is related to both the material and IDT. The IDTs were highly reflective and created mainly standing waves, both under the IDT region and within the propagation region.

In order to properly build an acousto-electronic transport device with silicon, suitable and high quality piezoelectric material is indispensable. Dedicated material deposition tools inside a cleanroom (preferably in-house) are needed, with many rounds of optimization for specific device use. Materials not so specialized can only be of limited application and use.

To further examine the nature of the material source of SAW attenuation, an analysis of the effect of a very thin amorphous SiO₂ capping layer on pristine single-crystal lithium niobate on SAW propagation will be shown in the next chapter.

HIGH-FREQUENCY ACOUSTIC PROPAGATION LOSSES IN SiO_2 ON LiNbO_3

4.1 INTRODUCTION

Single-crystal substrates are the material of choice for piezoelectric acoustic applications [9, 41]. In single-crystal materials, assuming perfect SAW generation, propagation loss can be limited to phonon scattering within the substrate and losses due to gas loading [42–45]. However, further functionalization of piezoelectric materials or interfacing them with other substrates like silicon requires additional processing and in most cases additional material layers [28, 46]. In acousto-electronic transport experiments propagation loss of acoustic waves is a limiting factor for device operation (see Chapter 2).

Thin films deposited on piezoelectric substrates can have beneficial effects, such as temperature compensation of SAW frequencies by using silicon dioxide layers [47–50]. On non-piezoelectric substrates such as silicon, the deposition of piezoelectric thin-films can also lead to higher SAW frequencies via the higher acoustic velocities of the substrate [33]. However, because additional layers can have a different speed of sound, can be amorphous, and add mass on top the substrate, their electrical and mechanical impact on surface acoustic wave (SAW) generation and propagation can not be neglected [51–54].

4.2 EXPERIMENTAL

4.2.1 Device structure

In this work, we fabricate delay lines on a single-crystal 128°Y -cut lithium niobate (LiNbO_3) 100 mm wafer using nano-imprint lithography. The delay lines consist of double-finger IDTs with a separation of $1,082\text{ }\mu\text{m}$ and $306\text{ }\mu\text{m}$. The wavelengths investigated are $1,000\text{ nm}$, 800 nm , 640 nm , and 520 nm , which correspond to finger sizes of 125 nm , 100 nm , 80 nm , and 65 nm , respectively [13]. Further, to examine the effect of a sputtered amorphous layer on the generation and propagation of SAWs, we also fabricated delay lines on

single-crystal 128°Y -cut LiNbO_3 with a sputtered capping layer of 20 nm of SiO_2 .

4.2.2 Vector network analysis

The X-axis of 128°Y -cut of lithium niobate has one of the highest electromechanical coupling coefficients (ca. $K^2 \approx 5\%$) and SAW velocities ($v_{\text{SAW}} = 3,979 \text{ m s}^{-1}$) of known piezoelectric materials for the fundamental SAW mode [9, 55]. In such a material, we can expect a sharp dip in reflection and reasonably high transmission at the resonant SAW frequency during VNA measurements of our delay lines.

Figure 4.1 shows the scattering parameters of $1,085 \mu\text{m}$ spaced delay lines for various wavelengths on both free and capped LiNbO_3 . There are well-defined features in both S_{11} and S_{21} for most wavelengths. To check the SAW velocity, we can take the SAW frequency of the $\lambda = 1,000 \text{ nm}$ delay line $f_{\text{SAW}} = 3.6 \text{ GHz}$:

$$v_{\text{SAW}} = \lambda \cdot f_{\text{SAW}} = 1,000 \mu\text{m} \cdot 3.6 \times 10^3 \text{ GHz} = 3.6 \times 10^3 \text{ m s}^{-1}. \quad (4.1)$$

This is lower than the expected literature value for the X-axis, which can be explained by a misalignment of the NIL stamp to the ideal wafer cut. The SAW velocity is closer to the theoretical velocity for the minor y-axis, which is perpendicular to the X-axis on the 128°Y -cut surface [55].

The transmissions for the DF delay lines in Fig. 4.1a, have many oscillations instead of a single peak. This is partially characteristic of SAW resonator behavior, as multiple reflections at the IDTs in the delay line create many standing waves between them. The period of the resonance oscillations seen in the transmission of the $\lambda = 1,000 \text{ nm}$ is around $\Delta f = 3 \text{ MHz}$, which corresponds to a cavity size L of:

$$L = \frac{v_{\text{SAW}}}{\Delta f} = \frac{3.6 \times 10^3 \text{ m s}^{-1}}{3 \text{ MHz}} = 1.2 \times 10^3 \mu\text{m}. \quad (4.2)$$

This is a cavity with a size of the delay line extending partially into both IDTs. If compared to a SAW resonator, the IDTs are acting as both exciting IDTs and Bragg mirrors. Depending on the reflectivity of the individual IDT fingers in such a resonator, the SAWs typically extend to about one half the length of the mirror [56]. All SAW transmission resonances in both free and capped LiNbO_3 have a beating frequency of about $\Delta f \approx 3 \text{ MHz}$, which correspond to a cavity size of $L \approx 1.2 \times 10^3 \mu\text{m}$.

The experimental values for SAW velocity and effective electromechanical coupling coefficient (extracted via method described in Ref. [10]) for the NIL delay lines are shown in Figure 4.2. The increase in frequency for smaller

Figure 4.1: Vector network analysis of double-finger NIL SAW delay lines on single-crystal 128°Y-cut LiNbO₃ with and without a SiO₂ capping layer. a) An overview of the SAW resonances excited by DF IDTs on free LiNbO₃. All four wavelengths exhibit high transmission with beating oscillations of the peak indicating resonant behavior of the delay line. The reflection resonance in S_{11} is a peak instead of a dip, indicating that the IDTs are great SAW reflectors and also highly impedance mismatched to the VNA. b) An overview of the SAW resonances excited on SiO₂ capped LiNbO₃. All four resonances also have peaks in reflection. The detected transmission power slowly decreases with wavelength, until finally it is only visible with time gating for $\lambda = 520$ nm (indicated by *).

Figure 4.2: Analysis of VNA measurements of NIL IDT delay lines on free and SiO_2 (20 nm) capped LiNbO_3 . Top segment shows measured frequency, middle: calculated velocity, and bottom: calculated experimental electromechanical coupling coefficient K^2_{exp} . While the frequency response of the IDTs increases with smaller wavelength as expected, the velocity decreases slightly. This can be an effect of increasing mass loading at smaller wavelengths (see Chapter 5). There is no clear trend in K^2_{exp} .

wavelengths is as expected and there is no appreciable difference between free and capped LiNbO_3 . The velocity decreases with smaller wavelengths, which is an effect of mass loading due to the IDT electrodes [57]. The velocity for capped LiNbO_3 is slightly lower than for the free surface, which is due to the lower SAW velocity in SiO_2 . The experimental electromechanical coupling coefficient K^2_{exp} is comparable to the value for the minor y-axis of a 128°Y -cut wafer surface [55].

For the case of a simple SAW resonator, one would still expect a dip in the reflection, indicating a conversion of electrical energy to mechanical via the inverse piezoelectric effect. The peak in the reflections S_{11} can be attributed to a highly electrically reflective IDT, with a large impedance mismatch from the conventional $50\ \Omega$. A further investigation on this matter will be carried out in Chapter 5. The additional small oscillations in the reflection may be due to further interactions of reflecting SAW waves within the IDT itself [7, 29].

Figure 4.3: VNA comparison of NIL SAW delay lines with different lengths. a) $\lambda = 520 \text{ nm}$ on LiNbO_3 . b) $\lambda = 520 \text{ nm}$ on $\text{SiO}_2 / \text{LiNbO}_3$. An increase in the SAW propagation loss $\alpha = \Delta S_{21} / (d_2 - d_1)$ is seen due to presence of a capping layer (see also Fig. 4.4).

4.2.2.1 Propagation loss analysis

Surface acoustic wave attenuation is described by a propagation loss α , which can be quantified by a measurement of the transmissions S_{21} for two delay lines of different length d [58, 59]:

$$\alpha = \frac{\Delta S_{21}}{\Delta d} [\text{dB mm}^{-1}]. \quad (4.3)$$

Figure 4.3 shows a comparison between the transmission parameters S_{21} of delay lines on free and capped LiNbO_3 for the wavelength $\lambda = 520 \text{ nm}$. The transmission is smaller for a delay line of greater length in both cases (red line). The difference in transmission, ΔS_{21} , increases by 4 dB for the capped substrate, showing more loss along the delay line due to the additional thin film SiO_2 cap.

Figure 4.4 shows a comparison of ΔS_{21} for two different wavelengths. As propagation loss is frequency dependent, there is more loss for shorter wavelengths (higher frequencies) from -13 dB mm^{-1} at $\lambda = 1,000 \text{ nm}$ to -19 dB mm^{-1} and -22 dB mm^{-1} at $\lambda = 520 \text{ nm}$ on the free and capped substrate, respectively. This is comparable to propagation loss in cut directions of single-crystal piezoelectric materials with weak SAW electromechanical coupling ($K^2 \sim 1 - 2\%$) and slow SAW velocities ($v < 4,000 \text{ m s}^{-1}$) [44].

There is also a frequency difference between the short and long delay line seen in Fig. 4.3. On both free and capped LiNbO_3 , the longer $1,085 \mu\text{m}$ delay

Figure 4.4: Propagation loss dependence on wavelength (frequency) in delay lines on LiNbO_3 . A comparison of delay lines with wavelengths of $\lambda = 1,000$ nm and 520 nm on free and capped LiNbO_3 . An increase in SAW propagation loss at smaller wavelengths (higher frequencies) is seen. The triple transit echo (TTE) is also shown for $\lambda = 1,000$ nm and shows a marked larger SAW propagation loss for larger distances on the capped substrate. There was no detected TTE for $\lambda = 520$ nm (see also Fig. 4.5).

line has a higher resonance frequency. The different resonance conditions within the delay lines is the likely origin, where constructive and destructive interference allows only slightly higher frequencies in the longer delay line. On the other hand, the NIL template could also be the source, as slight differences during its EBL fabrication may shift the individual IDT resonances slightly.

Included in the figure is a comparison of the *triple transit echo* (TTE) for $\lambda = 1,000$ nm. A triple transit echo is a SAW sent by the transmitting IDT and twice reflected by the receiving and transmitting IDT back to the receiver again. The direct transmission (up to 1,082 μm) shows only a small difference between free and capped substrate (in fact, the ΔS_{21} is smaller for the capped substrate, indicating a large measurement error). However, the TTE clearly shows a more pronounced loss for the capped substrate (from -13 dB to -20 dB). There was no detected TTE for $\lambda = 520$ nm, as the reflected SAW was most likely attenuated to below the noise level of the network analyzer. One can see a more complete picture in the time-domain traces of the SAW delay line.

4.2.2.2 Time-domain analysis

Figure 4.5 shows a comparison of the time-domain VNA measurements of $\lambda_{\text{SAW}} = 1,000 \mu\text{m}$ and $\lambda_{\text{SAW}} = 520 \mu\text{m}$ delay lines with an IDT separation of $l = 1,082 \mu\text{m}$ on LiNbO_3 and on $\text{SiO}_2(20 \text{ nm})/\text{LiNbO}_3$. Both time-domain traces in Fig. 4.5a show the characteristic first peak of the EM signal close to $0 \mu\text{s}$, followed by subsequent *delayed peaks* corresponding to SAWs. The first peak is the SAW originally sent by the transmitting IDT and detected by the receiving one. The following peaks can be attributed to subsequent multiple odd reflections and transits (in this case 3rd and 5th) [7, 13].

Immediately noticeable is the presence of all three peaks for the black trace (free lithium niobate) as opposed to only the first two for the red trace (with amorphous capping layer). Only the first SAW peaks are comparable in magnitude, whereas the following peaks decrease differently for the different substrates.

The second and third SAW peaks are more interesting for the purpose of demonstrating the effect of a thin amorphous layer on SAW propagation. Namely, both peaks are appreciably lower in magnitude on the capped substrate than on free lithium niobate and the third disappears altogether. One can also hypothesize, that the effect of such a layer becomes more appreciable with increasing thickness.

Additionally, the acoustic velocity of the SAW packages can be extracted from their time position. For the black trace, the start of the first peak is around $t_{\text{bare}} = 300 \text{ ns}$, corresponding to a velocity of $v_{\text{bare}} = 3.6 \times 10^3 \text{ m s}^{-1}$. For the red trace, the start of the first peak is around $t_{\text{cap}} = 280 \text{ ns}$, corresponding to a velocity of $v_{\text{cap}} = 3.8 \times 10^3 \text{ m s}^{-1}$. The black trace velocity matches well with the SAW velocity found above (Fig. 4.2), while the red trace velocity is higher. The SAW packet on the capped LiNbO_3 arrives sooner than on free LiNbO_3 . This is because the SAW resonance is broader in frequency on the SiO_2 capped substrate than on the free one (see $\lambda = 1,000 \text{ nm}$ in Fig. 4.1).

Figure 4.5b shows the time-domain comparison for $\lambda = 520 \text{ nm}$. The signal for the transmission on free LiNbO_3 is diminished as compared to $\lambda = 1,000 \text{ nm}$ and the transmission for the capped delay line is just above the noise level. As opposed to $\lambda = 1,000 \text{ nm}$, the SAW in the capped delay line is much slower than in the free surface device. Since the wavelength is smaller, the velocity of SiO_2 has a greater influence on the excited SAW due to a larger portion of the wave propagating within this slower film. There is no clearly visible TTE, however there are very small peaks present after the initial transmission which are attributed to noise.

In comparison to the $\text{SiO}_2/\text{ZnO}/\text{SiO}_2/\text{Si}$ multilayers in the previous chapters, it becomes clear that there is a trade off between multiple beneficial and detrimental effects; (i), the better the crystalline properties of the piezoelectric layer, the better the SAW propagation and vice versa (Fig. 3.6 vs. Fig. 4.1), (ii),

(a) comparison of $\lambda = 1,000$ nm (b) comparison of $\lambda = 520$ nm

Figure 4.5: Time-domain VNA comparison of NIL SAW delay lines on single-crystal 128°Y-cut LiNbO_3 and 128°Y-cut LiNbO_3 with 20 nm SiO_2 . a) comparison of time-domain VNA of $\lambda = 1,000$ nm IDTs. Signal loss is evident as compared to pristine LiNbO_3 (black) in the lower triple transit echo and non-visible quintuple transit echo (red). b) Time-domain VNA of $\lambda = 520$ nm IDTs. The red trace is lower than the black one and arriving at the second IDT.

surface material properties play a large role in the SAW properties even if the SAW penetrates into a single-crystal substrate (e.g. silicon in Fig. 3.6 or LiNbO_3 in Fig. 4.5), and finally (iii), the effect is greater at higher frequencies and larger delay line distances (following the frequency dependence of acoustic propagation loss [44]).

4.3 DISCUSSION AND CONCLUSION

In this chapter we have fabricated and analyzed NIL IDT delay lines on a 128°Y -cut LiNbO_3 substrate. To examine the effect of SAW attenuation due to additional material layers, a thin film of SiO_2 was sputtered on lithium niobate for comparison.

We showed large propagation loss at high frequencies on free LiNbO_3 , which only increased when the substrate was capped. A network vector analysis revealed a propagation loss increase from 19 dB mm^{-1} to 22 dB mm^{-1} due to the added 20 nm of SiO_2 for $\lambda = 520 \text{ nm}$ ($f_{\text{SAW}} = 6.8 \text{ GHz}$). Further, we showed the influence of propagation loss due to sputtered media via a time-domain analysis of the traveling SAWs in the delay lines. The capping layer was shown to have a larger attenuation effect, particularly on transit echos of the reflected SAWs.

The IDTs themselves are highly reflective, most likely due to their high number of finger pairs, causing resonator behavior within the delay lines. The additional capping material did not improve IDT electrical behavior. Since traveling waves, not standing waves, are needed for acousto-electronic transport, the IDT reflectivity must be reduced via proper electrical impedance matching the the RF power source.

In conclusion, deposition of thin films, such as SiO_2 capping layers, onto (piezoelectric) single-crystal substrates, introduces more loss for propagating surface acoustic waves. Further, when the piezoelectric layers themselves are thin films, which can have many imperfections, the propagation loss can be even larger. For silicon acousto-electronic devices, there is clearly a trade-off between functionalization and the introduction of more SAW scattering sources. The most straight-forward, perhaps less practical approach, would be optimization of both processing and piezoelectric material deposition for one specific application rather than general usage. Target frequencies can be limited to $< 10 \text{ GHz}$, which enables larger wavelengths and thicker piezoelectric films of better quality to be used. The processing can be adapted such that the piezoelectric material is added only in the last steps, which limits exposure to chemical and mechanical degradation. This middle-of-the-road approach can be more advantageous for future ACT experiments.

IMPEDANCE MATCHING FOR NIL SAW DEVICES

5.1 INTRODUCTION

Propagating surface acoustic waves (SAWs) are necessary for acousto-electronic *transport* experiments [22]. To obtain a useful propagating SAW, an interdigitated transducer (IDT) with a large electromechanical coupling to the substrate and a large acoustic transmission out of the IDT into the propagation region are desirable. At low temperatures, high-frequency SAWs (> 5 GHz) are needed to get above the thermal noise limit ($hf \gg k_B T$) in quantum-transport devices [32]. A good rule of thumb for efficient free-charge carrier capture and transport is that the carrier drift velocity v_d is equal to or greater than the SAW velocity v_{SAW} [25]. Since drift velocity is dependent on the carrier mobility μ and the electric field E , $v_d = \mu E$, in the case of low carrier mobility, a higher electric field can compensate to satisfy the velocity requirement. Higher-order-mode SAWs, in addition to having higher resonant frequencies, generate a higher electric field within the substrate than fundamental modes due to the waveguiding effect and thus, are capable of capturing and dragging charge carriers with a lower mobility [33]. Our goal in this chapter is to investigate the design of electrically and acoustically impedance matched IDTs, which excite traveling high-frequency and higher-order mode SAWs efficiently.

5.2 NUMERICAL SIMULATIONS OF IDTs

Numerical simulations offer a relatively straightforward way of designing RF IDTs on thin-film, multi-layered piezoelectric substrates [60]. Here, we use 2D numerical finite-element simulations in COMSOL Multiphysics to find grating SAW eigenfrequencies f_0 , which correspond to SAW velocities $v_{SAW} = \lambda_{SAW} / f_0$, of piezoelectric thin-film multilayers on a silicon substrate (Section 5.2.1). The eigenfrequencies are used to obtain the SAW electromechanical coupling constant K_{sim}^2 , which is substrate-specific, and is shown in Section 5.2.2. To find the IDT impedance (Z_{IDT}) on the simulated substrate, an equivalent-circuit model is introduced in Section 5.3. This model is dependent

on the IDT design specifications, the substrate material, and the calculated K_{sim}^2 . A comparison between model and experimental results (from Chapter 3) is shown in Sections 5.2.1 and 5.4.2. And finally, the limitation of the numerical simulations and equivalent-circuit model are discussed in Section 5.5.

5.2.1 ZnO multilayers

We chose to analyze a $\text{SiO}_2/\text{ZnO}/\text{SiO}_2$ thin-film stack on silicon. This configuration is known for producing higher-order SAW modes due to the waveguiding effect from the combination of the higher-velocity substrate and the insulating SiO_2 layers. Silicon dioxide also has a negative temperature coefficient of frequency (TCF), as compared to ZnO, which has a positive one. Thus, SAW resonance frequencies can be only weakly temperature-dependent with a balanced layer-thickness ratio [61]. This is beneficial for acousto-transport experiments at low temperature (as seen in Chapter 2). An overview of the material constants used in the COMSOL model is given in Appendix B.

Figure 5.1a shows the device structure in numerical simulations for a $\text{SiO}_2/\text{ZnO}/\text{SiO}_2/\text{Si}$ multilayer substrate with varying ZnO thickness h_{ZnO} , similar to devices in Chapter 3. The width of the structure is equal to the SAW wavelength λ_{SAW} and the boundary conditions are that of an infinite periodic structure. The black rectangles are electrodes with a set height of $h_{\text{el}} = 25 \text{ nm}$. A structure with two electrodes represents a single-finger device, however, the periodic boundary conditions actually make the simulated structure an infinite grating (Fig. 5.1b).

Figures 5.1c and 5.1d show an example of the calculated vertical displacement field within the substrate u_z at the SAW eigenfrequency f_0 for the symmetric mode and anti-symmetric mode, respectively. Together these two modes are considered the grating stop-band edges, $f_{\pm}$. [7, 60].

Calculated SAW velocities dependent on ZnO thickness are shown in Figure 5.2. As the ZnO thickness gets smaller, the SAW velocity increases due to the SAW penetrating deeper into the faster silicon substrate. The calculated velocities of SAWs in bulk material $v_{\text{SAW}}^{\text{material}}$ for the individual multilayers are marked in horizontal grey lines. Two SAW modes are visible, the fundamental mode R1 (the Rayleigh mode), and the first higher-order mode R2 (the Sezawa mode).

Velocities for mode R1 at large ZnO thickness approach that of bulk ZnO. In case of $\lambda_{\text{SAW}} = 260 \text{ nm}$, the velocity at high h/λ_{SAW} is slightly lower than $v_{\text{SAW}}^{\text{ZnO}} = 2,734 \text{ m s}^{-1}$. The reason is likely mass-loading due to a large electrode height and wavelength ratio $h_{\text{el}}/\lambda_{\text{SAW}}$, which we discuss in Section 5.5. The Sezawa mode R2 achieves higher velocities, approaching the bulk SAW velocity for silicon $v_{\text{SAW}}^{\text{Si}}$, due to the wave-guiding effect of the multilayer. For small h/λ_{SAW} the wave-guiding effect manifests as follows: the

Figure 5.1: Simulated periodic substrate structure with grating and examples of calculated SAW eigenfrequencies. a) Evaluated multilayer structure with varying ZnO thickness h_{ZnO} . Multilayer includes thin 20 nm SiO_2 capping layer (top yellow segment) and aluminium electrodes (black). b) A periodic grating and two different electrical conditions, open and short-circuited. Each case will result in two SAW eigenfrequencies such as in c) and d). The vertical displacement field u_z of the symmetric (c) and antisymmetric (d) SAW modes corresponding to grating stop-band edges, simulated here for $h_{\text{ZnO}} = 50$ nm and a periodicity of $\lambda_{\text{SAW}} = 400$ nm.

SiO_2 focuses the electric field within the piezoelectric layer, while the strain field couples to the underlying silicon, giving rise to a faster SAW mode [40].

For the wavelengths $\lambda_{\text{SAW}} = 1,000$ nm and 640 nm at very small h/λ_{SAW} , the simulated velocity surpasses that of the bulk silicon SAW velocity and approaches the bulk silicon transverse velocity $v_T^{\text{Si}} = 5,845$ m/s. These faster waves are still SAWs, but with the vertical-shear component suppressed within the thin piezoelectric film. At velocities greater than v_T^{Si} , SAWs become so called leaky SAWs, as a part of their component becomes coupled to bulk modes [7].

Figure 5.2: Calculated SAW velocities in ZnO multilayer via numerical simulation.

An overall trend of the velocity increasing with thinner h_{ZnO} can be seen, which corresponds to a larger SAW penetration into the faster silicon substrate. The faster velocity of mode R2 is due to the wave-guiding effect of the SiO_2 layers.

5.2.2 Electromechanical coupling constant

The effective electromechanical coupling constant K_{exp}^2 can be found experimentally from the absolute admittance $|Y_{11}|$ resonance f_r and anti-resonance f_a frequencies of a resonator. This can also be approximated via the velocities of a metallized v_{metal} and open v_{open} substrate [10]:

$$K_{\text{exp}}^2 \approx \frac{(f_r^2 - f_a^2)}{f_a^2} \approx \frac{(v_{\text{open}}^2 - v_{\text{metal}}^2)}{v_{\text{metal}}^2}. \quad (5.1)$$

However, to simulate the SAW resonance characteristics of an IDT we use a grating structure instead of a plain substrate (as seen in Section 5.2.1). This allows the model to incorporate the electrical and acoustic loading effects of the electrodes. The grating can have two electrical boundary conditions, open-circuited "OC" and short-circuited "SC". Both boundary conditions will each produce two resonances in the grating, the symmetrical f_+ and anti-symmetrical f_- (see Fig. 5.1), which correspond to the -3 dB band edges of

Figure 5.3: Calculated K_{sim}^2 from numerical simulations for two SAW modes for varying h_{ZnO} . a) R1 and b) R2. Evaluation of the propagation of SAWs in the ZnO multilayer substrate yields an ideal combination of SiO₂ and ZnO thicknesses. For R1, this corresponds to $h/\lambda_{SAW} = 0.3 - 0.4$ and for R2 to $h/\lambda_{SAW} = 0.4 - 0.45$. Grey line indicates h_{ZnO} used in experiments in Chapter 3.

the grating stopband. From Hashimoto [7], we use a K_{sim}^2 expression derived for finite-element methods for gratings:

$$K_{sim}^2 \approx \frac{\pi}{\eta^2} \frac{f_{OC-} + f_{OC+} - f_{SC-} - f_{SC+}}{f_{SC-} + f_{SC+}}, \quad (5.2)$$

where f_{OC} and f_{SC} are the open- and short-circuit grating resonance frequencies, respectively, and η is the element factor.

The element factor η is defined as the ratio of the excitation efficiency for each IDT finger pair relative to the best possible efficiency. It can be calculated theoretically from the charge distribution on the IDT electrodes, similar to the static capacitance C_S in later sections, and for the fundamental and first SAW harmonic excited by a single-finger IDT: $\eta = 0.84722[00]$ [7, 60].

Figure 5.3 shows the calculated coupling constant K_{sim}^2 of the first two SAW modes as a function of ZnO thickness h_{ZnO} for four different wavelengths. Due to the multilayer structure and the fast silicon substrate, mode R2 exhibits a higher coupling than R1. Such wave-guiding effects on higher-velocity substrates have been reported in literature since the 1970s and also recently in GaAs on LiNbO₃ [62, 63].

Normalizing h_{ZnO} by the wavelength, we obtain the ratio h_{ZnO}/λ_{SAW} . This allows us to observe that mode R1 has a shallow peak that is present around $h_{ZnO}/\lambda_{SAW} = 0.4$ for the wavelengths $\lambda_{SAW} = 260$ and 400 nm. Most likely the wavelengths $\lambda_{SAW} = 640$ and 1,000 nm will also have a maximum, but at a larger ZnO thickness. Mode R2 of all four examined wavelengths has

a peak in the coupling at around $h/\lambda_{SAW} \approx 0.4$, showcasing the benefits of the wave-guiding effect. An optimized piezoelectric layer thickness, via higher K_{sim}^2 , is necessary for better SAW generation at higher frequencies. We find an optimum ZnO thickness starting at $h/\lambda_{SAW} = 0.3 - 0.4$ for R1 and $h/\lambda_{SAW} = 0.4 - 0.45$ for R2.

5.3 IMPEDANCE MATCHING

An IDT on a piezoelectric substrate transforms an electric field into mechanical strain through the inverse piezoelectric effect. In this section we will use an equivalent-circuit model based on the work of Aref, et al. [32], which uses a 3-port network analysis of an acoustically transmitting IDT as its basis. Figure 5.4a shows the equivalent-circuit model of an IDT, which we use to determine its electro-acoustic behavior, superimposed on the numerically simulated substrate. Under RF power an IDT produces an acoustic response $\phi_{out}^\pm$, which has an equivalent load with a complex admittance $Y_a(\omega) = G_a(\omega) + iB_a(\omega)$. Additionally, an IDT has a static capacitance C_t , which also has a susceptance $i\omega C_t$, and together the IDT admittance can be expressed as [32, 64]:

$$Y_a(\omega) = G_a(\omega) + iB_a(\omega) + i\omega C_t. \quad (5.3)$$

At resonance $\omega = \omega_0$, the susceptance iB_a is zero and the real part of the admittance is only dependent on the radiation conductance at resonance $G_{a,0}$:

$$\text{Re}\{Y_a(\omega_0)\} = G_a(\omega_0) = G_{a,0}. \quad (5.4)$$

The extraction of $G_{a,0}$ from the model is non-trivial and is approximated by Aref [32] (based on Datta [29]). A different, yet complimentary approach, is followed by Smith [65], and the full determination from Maxwell's equations is given by Auld and Kino [66]. The final form is:

$$G_{a,0} = \frac{4}{\pi} K^2 N_p^2 \omega_0 C_S, \quad (5.5)$$

where K^2 is the electromechanical coupling constant, N_p is the IDT number of finger pairs, ω_0 is the angular resonance frequency, and C_S is the static capacitance of a single IDT finger pair, where $C_t = N_p C_S$ is that of the full IDT. From Hashimoto [7], the static capacitance is expressed as:

$$C_S = W\epsilon(\infty)\epsilon_0 \frac{P_{-1/2}[\cos(2\pi w/p_I)]}{P_{-1/2}[-\cos(2\pi w/p_I)]}, \quad (5.6)$$

where W is the IDT aperture, $\epsilon(\infty)$ is the effective permittivity of the substrate, P is a Legendre polynomial of the order $(-1/2)$, w is the IDT finger width and

Figure 5.4: Calculated impedance Z_0 of an equivalent-circuit for an electro-acoustic IDT. a) schematic of the circuit model of an IDT on a substrate. The calculated impedance Z_0^{sim} of b) R1 and c) R2 SAW modes using Equation (5.2). The IDTs are clearly not well matched to the periphery circuit standard of $Z_{ref} = 50 \Omega$ for any h_{ZnO} thickness. Grey line indicates h_{ZnO} used in experiments in Chapter 3.

$p_I = \lambda_{SAW}$ is the period of the IDT fingers. The argument in the Legendre function is the metallization ratio $2w/p_I$, which is the fraction of the substrate under the IDT that is metallized. The metallization ratio is equal to zero for a free substrate, 0.5 for a standard finger-spacing and one for a fully metallized substrate [7].

The admittance has to satisfy $Z_{ref} = 1/G_{a,0} = 50 \Omega$ in order to match the reference impedance Z_{ref} of the peripheral circuit. Thus, there is an inverse relation between the target impedance and the parameters of Equation (5.5). The following method is used to satisfy the condition for an impedance match. For a specific substrate with C_S and SAW wavelength λ_{SAW} , the IDT resonance frequency ω_0 and coupling constant K_{sim}^2 are numerically calculated. Then the aperture W and N_p are designed to meet $Z_{ref} = 50 \Omega$. The relation between the $G_{a,0}$ parameters themselves is also inverse, e.g. as the K_{sim}^2 rises, the ideal number of IDT finger pairs lowers.

For our nano-imprint IDT fabrication we use a stamp mask design with a fixed number of finger pairs N_{stamp} , metallization ratio $2w/p_I = 0.5$, and aperture $W_{stamp} = 30 \mu\text{m}$ (an overview can be seen in Table B.4). The design is not optimized for impedance, but rather as a test of the fabrication principle and thus, we can expect a large impedance mismatch. With N_p , $2w/p_I$, and W fixed for the stamp, the only parameter that can change is the material dependent C_S .

For our chosen thin-film multilayers on silicon, the calculated real part of the impedance at resonance Z_0^{sim} dependent on ZnO thickness h_{ZnO} is shown in figures 5.4b and 5.4c. The calculation is done using Equation (5.2) and K_{sim}^2

values seen in Fig. 5.3 for SAW modes R1 and R2. Both modes show a lower impedance than Z_{ref} , with only the largest wavelength $\lambda_{SAW} = 1,000$ nm of mode R1 yielding an impedance approaching 50Ω at small ZnO thickness. The calculated impedance for mode R2 is quite low ($< 5 \Omega$) due to a high coupling constant K_{sim}^2 , which is ten times higher than mode R1 (Fig. 5.3). While challenging in fabrication, the stamp design simply has too many finger pairs to achieve an impedance match.

The ideal number of finger pairs N_{ideal} , that the nano-imprint IDTs should have for impedance matching to Z_{ref} is,

$$\frac{1}{50[\Omega]} = \frac{4}{\pi} K^2 N_{ideal}^2 \omega_0 C_S,$$

$$N_{ideal} = \sqrt{\frac{1}{50} \frac{\pi}{4 K^2 \omega_0 C_S}}. \quad (5.7)$$

For experimental samples in Chapter 3, the substrate thin-film thickness was optimized for second mode SAW generation by making the thermal oxide $h_{SiO_2} = 100$ nm and $h_{ZnO} = 100$ nm and thus, fixing also C_S in Equation (5.7). An overview of the calculated impedance values and ideal number of IDT finger pairs N_{ideal} for the experimental samples is shown in the Appendix B.

5.4 COMPARISON TO EXPERIMENTAL VALUES

5.4.1 ZnO multilayers on silicon

Impedance Z of an IDT is examined experimentally by vector network-analyzer (VNA) measurements of the complex reflection parameter S_{11} :

$$Z_{11} = Z_{ref} \left(\frac{1 + S_{11}}{1 - S_{11}} \right) = R_{11} + iX_{11}, \quad (5.8)$$

where Z_{ref} is the reference impedance of the VNA ($Z_{ref} = 50 \Omega$), and the complex impedance components, the real resistance R_{11} and the imaginary reactance X_{11} [7].

Figure 5.5 shows the complex impedance components of nano-imprint IDTs on ZnO/Si multilayers from Chapter 3. The nano-imprint IDTs come in two types, single-finger IDT with $\lambda_{SAW} \leq 500$ nm and double-finger (DF) IDTs with $\lambda_{SAW} \geq 520$ nm. Resistance R_{11} in both Fig. 5.5a and 5.5b is below the impedance standard with only $\lambda_{SAW} = 520$ nm approaching 50Ω at higher frequencies. Reactance X_{11} is non-zero in both cases, with only double-finger IDTs in Fig. 5.5a crossing the zero level. Mode R2 of $\lambda_{SAW} = 1,000$ nm has a reactance close to $X_{11} = 0$, however, R_{11} is at the furthest point from 50Ω in

Figure 5.5: Measured components of IDT resonance resistance R_{11} and reactance iX_{11} on ZnO/Si multilayers from Chapter 3. VNA complex scattering parameter S_{11} can be transformed into real and imaginary components of the IDT complex impedance Z_{11} . All experimental values of the resistance R_{11} are less than the impedance $Z = 50 \Omega$ of the VNA, resulting in a large imaginary reactance X_{11} .

the frequency scan, since a zero-crossing of the reactance corresponds to a minimum of the resistance.

Positive or negative reactance compares to capacitive and inductive IDT behavior, respectively. Large reactance is not desirable, since inductive or capacitive behavior implies that energy is stored in the near field (electric field for capacitor and magnetic for inductor) rather than being converted into energy carried by the SAW. Hence, reactance close to zero (an IDT will always have a small $\sim \text{pF}$ parasitic capacitance, as seen from element $i\omega C_t$ in Equation (5.3)) and a resistance identical to $Z_{ref} = 50 \Omega$ to eliminate reflections is ideal.

An overview of the impedance complex component values for selected SAW modes can be found in Figure 5.6. Impedance values are needed to properly

Figure 5.6: Performance of NIL IDTs on ZnO/Si multilayer from Chapter 3. Top: IDT complex impedance Z_{11} components extracted from VNA scattering parameter S_{11} . All experimental values of the resistance R_{11} are less than the reference impedance $Z_{ref} = 50 \Omega$. Bottom: K_{exp}^2 values extracted from $|Y_{11}|$. R2 modes show a higher coupling than R1 modes. Dotted lines are guides to the eye. All extracted impedance values for SAW modes can be found in Appendix B.3.

match an IDT or RF filter to any external circuits with appropriate additional electronic components.

The performance of an IDT can also be assessed by experimentally determining the coupling constant K_{exp}^2 via extraction of f_r and f_a from the IDT admittance (Equation (5.1)). Figure 5.6 shows the values of the complex impedance and electromechanical coupling constant extracted for modes R1 and R2 from ZnO/Si multilayer delay-lines seen in Figure 5.5. All extracted impedance values for SAW modes can be found in Appendix B.3.

As is immediately noticeable in the top part of Figure 5.6, the simulated resistance is much smaller compared to the experimental one. This is a result of the basic simulation setting of an isolated, transmitting IDT, while fabricated IDTs are always connected to a peripheral circuit (bus-bars, co-planar waveguide leading to contact pads and probes with leads to VNA). Additionally, the IDT equivalent-circuit model was that of a single IDT with infinite media on both sides [32]. The fabricated IDTs, on the other hand, were in a formation with several delay-lines after one another [13]. When the silicon sample edges are included, the S_{11} by the VNA resembles that of a long, many-IDT resonator. Such complex IDT structures and the corresponding coupling-of-modes models have been explored in the RF filter industry and a good introduction can be found in Hashimoto [7].

Numerical simulations predict that mode R2 has a higher coupling constant than R1. This is seen as a more pronounced dip in the reflection S_{11} in VNA measurements for R2 than R1 (seen also as resistance peaks in Figure 5.5). The lower part of Figure 5.6 compares the numerical K_{sim}^2 and experimental coupling constant K_{exp}^2 calculated from VNA reflection values. For single-finger IDTs ($\lambda_{\text{SAW}} \leq 500$ nm), K_{exp}^2 for mode R2 is higher than mode R1, as expected, although all numerical values are lower than experimental ones. There is a small rising trend in K_{exp}^2 for smaller wavelengths for both SAW modes. This trend is only seen for mode R2 in numerical values. For double-finger IDTs ($\lambda_{\text{SAW}} \geq 520$ nm), the experimental values do not show a clear higher value for mode R2. While for mode R1 the experimental values are higher than numerical ones, for mode R2 they are closer and also comparable for two SAW wavelengths.

The disparity between experimental and simulated values in SF and DF IDTs is a consequence of the different internal reflections of SAWs within the two different experimental IDT types. Alternatively, since the single- and double-finger IDTs were fabricated on ZnO multilayers deposited by two different methods, this can simply be of material origin. The difference between experimental and numerical values for K^2 in general, is from the limited nature of 2D FEM simulations, especially at small $h_{\text{ZnO}}/\lambda_{\text{SAW}}$ values where mass-loading effects increase. Further, in the case for SF IDTs, the shape of the resonances in Z_{11} are quite wide and thus, extraction of f_r and f_a is more prone to errors. This is also why K_{exp}^2 for $\lambda_{\text{SAW}} = 320$ nm is lower than for 260 nm or 400 nm in mode R2. An overview of the calculated and experimental IDT performance values is shown Table B.4 and B.6, respectively.

5.4.2 LiNbO₃ substrates

Impedance components R_{11} and X_{11} are extracted from scattering parameters for IDT delay-line devices on LiNbO₃ from Chapter 3. The IDT performance is shown in Fig. 5.7 and 5.8 for free and capped LiNbO₃, respectively.

For wavelengths $\lambda_{\text{SAW}} \leq 500$ nm (single-finger IDTs), the experimental impedance values shown in the upper segment of Fig. 5.7 are close to 50Ω , while wavelengths $\lambda_{\text{SAW}} \geq 520$ nm (double-finger IDTs) have a larger impedance mismatch. Numerical simulations show no agreement in resistance R_{sim} at resonance to experimental R_{11} . In fact, all calculated resistance values are on the order of ~ 10 m Ω , indicating very large internal reflection. This mismatch is verified experimentally by the shape of the resonance reflection S_{11} in Figure 4.1, i.e. the resonance is a peak instead of the expected dip. The larger experimental impedance values than calculated ones are most likely from the limited nature of the numerical model.

Figure 5.7: Performance of NIL IDTs on single-crystal 128°Y-cut LiNbO₃ from Chapter 3. Top: IDT complex impedance Z_{11} components extracted from VNA scattering parameter S_{11} . All experimental values of the resistance R_{11} are less than the reference impedance $Z_{ref} = 50 \Omega$. Bottom: K_{exp}^2 values extracted from $|Y_{11}|$. Numerical simulations for R_{sim} and K_{sim}^2 are shown for comparison. Dotted lines are guides to the eye.

The electromechanical coupling constant K_{exp}^2 is shown in the lower segment of Fig. 5.7 and is higher for single-finger IDTs than for double-finger IDTs. This can be a consequence of the large impedance mismatch shown in the top segment. Simulations also show a higher $K_{sim}^2 > 6\%$ than for both literature (5.5% [55]) and experimental values ($\sim 1 - 4\%$, see Fig. 5.7). The coupling constant was calculated using f_{sym} values with Equation (5.1) rather than Equation (5.2). When Equation (5.2) is used, the obtained coupling constant is even higher ($\sim 13\%$). However, simulations for larger wavelengths ($\lambda_{SAW} > 10 \mu\text{m}$) show a gradual decrease of the coupling constant to a value comparable to literature. When the LiNbO₃ substrate is simulated without IDT electrodes, but using the free and metallized surface velocity values, the calculated K_{sim}^2 is also close to literature values. This is clearly an effect of mass-loading of the electrodes and for small wavelengths the simulations are more erroneous. A denser FEM mesh does not correct this discrepancy and thus, this highlights a limitation of 2D FEM modeling of SAW devices with small wavelengths as infinite gratings.

Figure 5.8 shows the performance of IDTs on LiNbO₃ with a 20 nm capping layer of SiO₂. There is an additional SAW mode at a higher frequency, which is

Figure 5.8: Performance of NIL IDTs on single-crystal 128°Y-cut LiNbO₃ with capping layer from Chapter 3. Top: IDT complex impedance Z_{11} components extracted from VNA scattering parameter S_{11} . All experimental values of the resistance R_{11} are less than the reference impedance $Z_{ref} = 50 \Omega$. Bottom: K_{exp}^2 values extracted from $|Y_{11}|$. Numerical simulations for R_{sim} and K_{sim}^2 are shown for comparison. Dotted lines are guides to the eye.

labeled as R2, which is present due to the additional material on LiNbO₃. As in the case for free LiNbO₃, fabricated IDTs show a large impedance mismatch to 50Ω and between the simulated values of the resistance at resonance R_{sim} are very small ($\sim 10 \text{ m}\Omega$).

The electromechanical coupling constant for the first mode R1 is again higher for the simulated substrate than measured experimentally. This can be a result of an error in the extraction of f_r and f_a , due to the weak resonance signal in S_{11} . Furthermore, the experimental value of K_{exp}^2 for mode R2 is similar to that for R1 at $\lambda_{SAW} = 520$ and $1,000 \text{ nm}$ (about 1 %), while it peaks at about 5 % at $\lambda_{SAW} = 800 \text{ nm}$. The second mode is not seen in 2D numerical simulations, which are limited to the (x,z) orientation. This indicates that mode R2 can be a shear-horizontal SAW mode (Love mode), propagating along the (x,y) plane. Both modes have a peak in the reflection scattering parameter S_{11} as seen in Figure 4.1b. We take this to mean the IDTs are highly reflective electrically and acoustically due to their long length (high N_p). A complete overview of the calculated IDT performance parameters for both free and capped LiNbO₃ is shown in Table B.5 and an overview of the experimental IDT performance values is shown in tables B.7 and B.8

5.5 MASS LOADING

As the SAW wavelength decreases, the surface material properties have a greater influence on its generation and propagation due to the fact that the SAW is more localized to the surface. One of the effects of additional material on a surface is mass-loading.

Mass loading is the change of propagation velocity of SAWs due to the addition of material through which the SAW has to travel. For an IDT, mass-loading depends on both the thickness and the density of the electrode. Hence, mass-loading is more pronounced for thicker electrodes of the same material or for electrodes consisting of heavier metals (e.g. Au versus Al). The greater the change in velocity, the more surface waves will reflect at this discontinuity.

5.5.1 Effect within an IDT

Figure 5.9 shows the normalized difference of the calculated symmetric and anti-symmetric resonance frequencies, $\Delta f / f^{sim} = (f_{0,sym} - f_{0,asym}) / f_{0,sym}$, for two different electrode heights $h_{el} = 25$ nm and 40 nm. The impact of thicker IDT electrodes on the resonance frequencies of a metal grating is calculated for different wavelengths (left) and different h_{ZnO} (right). The effect is more pronounced for smaller wavelengths, as seen in the top segment. The normalized ratio h_{el} / λ_{SAW} for an electrode height of 40 nm and a wavelength of 260 nm is close to ~ 0.15 . This is quite high, as the standard is around ~ 0.01 to prevent unwanted wave reflections [67]. On the other hand, in some specialized cases the reflective nature of the electrode thickness can be desirable, e.g.: for spurious mode suppression [57, 68].

The right segment of Fig. 5.9 highlights the mass-loading effect by a thin piezoelectric material under an IDT, as it is the case for the $\text{SiO}_2/\text{ZnO}/\text{SiO}_2/\text{Si}$ multilayer. Here, the SAW is concentrated into the top part of the thin-film multilayer and thus, the influence of the electrodes is more pronounced. Increasing Δf is most likely the source of the small dip in K_{sim}^2 for the smallest wavelength 260 nm in the lower part of Fig. 5.6. Mass loading has a detrimental effect on an IDT's performance and can be minimized by thinner electrodes or even special IDT configurations (Chapter 7).

5.5.2 Effect outside IDT

An IDT-based device, such as a delay-line, consists of two types of surfaces; the partially metallized surface of an IDT and the free surfaces next to the IDT. Figures 5.10 a) and b) show the calculated eigenfrequencies f_0 for $\lambda_{SAW} = 260$ nm of a free surface and a fully metallized ($h_{metal} = 25$ nm), respectively. The calculated frequency difference is quite large $\Delta f \approx 300$ MHz.

Figure 5.9: Grating stop-band edge difference Δf as a function of electrode h_{el} and ZnO thickness h_{ZnO} . The numerical simulations yield two modes for each Rayleigh wave: symmetrical and anti-symmetrical, as seen in Fig. 5.1. The separation in frequency space of the two modes for R1 rises for thinner ZnO layers and smaller wavelengths and is a consequence of mass-loading.

From Equation (5.1) a higher velocity difference between a metallized and a free surface corresponds to a larger K^2 . However, SAW transmission can be hindered when taking into account the wave reflection at the interface between the two types of surfaces.

In the equivalent-circuit model, this can be expressed as [7]:

$$Z_a = \frac{1}{f C_T K^2}. \quad (5.9)$$

In order to compare the reflection Γ at the interface one can use the formula for electrical reflection:

$$\Gamma = \frac{Z_1 - Z_2}{Z_1 + Z_2}, \quad (5.10)$$

where Z_1 and Z_2 are the impedances of the relevant regions.

Figure 5.10c shows a sketch of a delay-line with high velocity differences between areas. In such a situation, the SAW generated by the left IDT is partially reflected at the inner IDT edge. When the SAW transmitted into the propagation region (middle) reaches the right IDT, it gets partially reflected again. This results in standing waves and the system behaves as several resonating cavities in series. This most likely explains the S_{11} measurements for delay-lines on LiNbO_3 substrates in Chapter 4, which had peaks in the reflection S_{11} instead of dips.

Figure 5.10: Eigenfrequency difference for the R1 SAW mode for substrates with and without metal. a) and b) Electrical and mechanical properties result in different SAW eigenfrequencies for substrate areas with and without metal (shown for $\lambda_{SAW} = 260$ nm). c) In a delay-line, a SAW is generated within an IDT (a partially metallized area). A large mismatch in acoustic frequencies to the free substrate can result in low SAW transmission out of the IDT. The large SAW reflection within the IDT area leads to a predominantly standing wave, similar to a one-port resonator.

5.6 DISCUSSION AND CONCLUSION

In this Chapter we used finite-element simulations to analyze the electro-acoustic behavior of IDTs. We investigated IDT acoustic performance by estimating the electromechanical coupling constant K_{sim}^2 for substrates with various thin-film layer thickness and composition. We determined IDT electrical compatibility to a peripheral circuit via their theoretical impedance Z_0 at resonance f_0 . And finally, we compared these parameters to experimental values extracted from VNA measurements of IDT delay-lines fabricated with nano-imprint lithography.

We find the ideal ZnO layer thickness h_{ZnO} in a ZnO/Si multilayer for selected wavelengths to be around $h/\lambda_{SAW} \sim 0.4$ for the first higher-order SAW mode R2, which agrees well with literature. We determine that our existing IDTs are too long, with a high number of finger pairs N_p , making them very

reflective, both electrically ($Z_0 \neq 50 \Omega$) and acoustically ($Z_{IDT} \neq Z_{substrate}$). This makes delay-lines fabricated with N_{stamp} behave as many-port resonators by promoting the presence of standing waves within and between the IDT region. Additionally, for small wavelengths ($\lambda_{SAW} \leq 400 \text{ nm}$), we identify an additional factor promoting reflection of SAWs, namely mass-loading from the IDT electrodes. And lastly, using the calculated value of K_{sim}^2 we estimate the ideal number of IDT fingers (N_{ideal}) for correct matching to 50Ω .

Comparing calculated and experimental IDT performance parameters, we find that our simple 2D model is insufficient to fully replicate the complex behavior of highly reflective delay-lines. Naturally, an acousto-electronic transport device needs propagating SAWs and not standing waves to function properly. Therefore, impedance matching IDTs not only to the peripheral circuit, but also designing them so that they do not form resonating structures is crucial. For a more complete model, which includes material, interface effects, and distant devices, we refer the reader to excellent work by Plessky and Koskela, 2000 [69].

THIN-FILM ScAlN WITH NIL FOR UHF SAWs

6.1 INTRODUCTION

Thin-film piezoelectric materials enable access to high frequencies (>5 GHz) for acoustic applications [33]. Aluminum nitride is especially attractive for its high acoustic velocity ($\sim 5,800 \text{ m s}^{-1}$, see Table 6.1), compatibility with CMOS integration [46] and mechanical material robustness [70]. Recently, Sc-doped AlN is vigorously investigated due to its stronger piezoelectric coupling enabling high-performance application in RF filters [71–73].

In this chapter, we use nano-imprint lithography (NIL) to fabricate acoustic devices with feature sizes down to 65 nm enabling the investigation of the performance of ScAlN thin-films on silicon material performance at high frequencies.

6.2 SAMPLE STRUCTURE AND DEVICE FABRICATION

As a substrate we use a double side polished, lightly p-doped (100) silicon wafer ($5 - 10 \Omega \text{ cm}$, diameter 100 mm, *Okmetic*) which is first thermally oxidized at $1,050^\circ\text{C}$ to grow a 100 nm thin-film of silicon dioxide. The wafer is then diced into 45×45 mm pieces and cleaned using an acetone/IPA/DI water ultrasonic procedure. Deposition of the piezoelectric material ScAlN is carried out by *Instituto de Sistemas Optoelectrónicos y Microtecnología*, at *Universidad Politécnica de Madrid*, Spain (see Ref. [74]) with target thicknesses of 300 nm and 100 nm. The wafer pieces are cleaned again before thin-film deposition and after transport back to *NanoLab*, University of Twente.

Nano-imprint lithography is used to define and fabricate interdigitated transducers (IDT) in a delay-line configuration (see fig. 1.4 or Appendix in Ref. [28]). In Figure 6.1a, an imprinted wafer piece can be seen on a carrier wafer. In order to properly align the imprints onto a non-standard wafer piece, a carrier wafer was first imprinted. Then the wafer piece is adhered to the carrier wafer with water or photo-resist and using slight adjustments aligned to the imprints. The wafer piece can then be imprinted. In Figure 6.1a,

Figure 6.1: Nano-imprint lithography of IDT delay-lines a) Image of an imprinted substrate on a Si carrier wafer. Changes of coloring within an imprint indicate presence of particulates on the surface. b) An optical microscope image of an IDT edge with thick contact pads. c) SEM image of double-finger IDT fingers, feature size is 65 nm.

the wafer piece has eight imprints, while the carrier wafer has four more, which were used for the imprint targeting. Note the changing color of the imprints on the wafer piece as opposed to the more uniform imprints on the carrier wafer. This indicates a variation of thickness in the imprint resist due to the imperfect landing of the NIL template. The origin is mainly surface contamination with particles which prohibit a level imprint of the template. The presence of the carrier wafer only exacerbates the uneven leveling of the substrate to the template, prompting more imprint resist use and further imprint imperfections.

Imperfect imprinting notwithstanding, fabrication proceeded and some IDTs were able to be successfully fabricated as seen in Figures 6.1b and 6.1c. The IDTs are metallized by e-beam evaporation with a Ti/Al/Ti (5/15/10 nm) stack. Thicker Al (100 nm) IDT contact pads were also evaporated in a subsequent photo-lithography step.

The fabricated IDTs are double-fingered with feature sizes of 125, 100, 80, and 65 nm, corresponding to surface acoustic wave wavelengths 1000, 800, 640 and 520 nm, respectively. A schematic of the substrate structure with fabricated delay-line specifics are given in Figure 6.2.

6.3 DEVICE CHARACTERISATIONS

The fabricated IDTs are contacted in a probe station using ground-signal RF probes up to 40 GHz from *Picoprobe* connected to an *Agilent PNA-X N5244A* vector network analyzer with time-domain analysis feature. The network analyzer was calibrated before measurement using an electronic calibration module in the short, open, load (50 Ω), through (SOLT) configuration.

Figure 6.2: Sample substrate and schematic of investigated delay-line devices. a) The device substrate is lightly p-doped Si (100) with 100 nm thermal SiO_2 and the active layer $\text{Sc}_{0.26}\text{Al}_{0.74}\text{N}$ in two thicknesses 100 nm and 300 nm. b) The NIL delay-line schematic. The IDTs are nominally identical and their length is $300 \mu\text{m}$.

6.3.1 300 nm ScAlN

Figure 6.3 shows the scattering parameters of delay-lines on the 300 nm ScAlN thick sample. Immediately visible are the higher-mode resonances in the reflection, which have a corresponding peak in the transmission, showing very good SAW propagation. There is a gradual decrease in signal strength for the R2 mode with higher frequency, which can be attributed to intrinsic frequency-dependent scattering (viscous damping) [44].

The fundamental Rayleigh mode is quite weak and only present for the 1000 and 800 nm wavelengths in the reflection and not at all visible in the transmission. The reason for this is not clear, but may be due to the combination of small wavelengths and fast velocity thin-film on slow substrate. Further, there is a wide high-frequency bulk acoustic wave mode seen in the transmission, which is most likely excited by the large contact pads next to the IDT and is a common spurious IDT response [7].

For time-domain analysis, the frequency window was set to 300 MHz around the resonance examined and the frequency scanning step to 30 kHz. A time-domain analysis of the higher mode R2, seen in Fig. 6.4, shows the mode is actually comprised of two distinct waves arriving at ca. 200 and 300 ns at the receiving IDT. The second component is most likely a transverse wave generated by the IDT. Usually, these spurious modes are less powerful than the primary Rayleigh modes. However, here it is not the case and the second wave is the only one measured for the smallest wavelength 520 nm. This can be due to the combination of "fast on slow" acoustic materials making the acoustic wave have a more transverse characteristic [75], in addition to concentration (waveguide effect) of the SAW strain field within the $\text{ScAlN}/\text{SiO}_2$ layer. The effect is most likely thickness dependent on both ScAlN and SiO_2 . The triple transit echo (TTE) is detected only for the largest wavelength (1,000 nm) and

Figure 6.3: Vector network analysis of NIL delay-lines on 300nm ScAlN/100nm SiO₂/Si. Large dips in the reflection correspond to the SAW R2 mode. The transmission shows additional wide frequency peaks after the R2 mode, most likely from BAWs.

Figure 6.4: Vector network time analysis shown in Figure 6.3. Shown are the times of arrival of SAWs on the receiving IDTs in S_{21} . For the wavelength $\lambda = 1,000$ nm (shown in blue), the incident SAW arrives at $t \approx 200$ ns, with the triple reflection following at $t \approx 600$ ns. Additionally, a time-domain of the sending IDT S_{11} for the $\lambda = 1,000$ nm is also shown on top (black). Here, the reflected wave is registered coming back at around $t \approx 400$ ns, which matches the behavior seen in S_{21} .

Table 6.1: Material acoustic wave velocities. The velocities of acoustic waves for materials used in this chapter, where v_{SAW} is the surface acoustic wave velocity in bulk material, $v_l = \sqrt{C_{11}/\rho}$ the bulk longitudinal velocity and $v_t = \sqrt{C_{44}/\rho}$ the bulk transverse velocity. AlN is added for comparison. All values are calculated using parameters from tables in Appendix C.

material	v_{SAW}^{*1} [m s ⁻¹]	v_l [m s ⁻¹]	v_t [m s ⁻¹]
AlN (002)	5800	11266	6220
Sc _{0.26} Al _{0.74} N	4765	9480	5246
SiO ₂	3300	5779	3643
Si	5083	8433	5844

*1 calculated using COMSOL Multiphysics.

is quite wide as compared to the first signal. The time broadening is due to the IDT transmitting a broad SAW package in time and these can only be distinguished at larger travel distances.

The acoustic wave velocities for the materials used in this work are shown in Table 6.1. AlN is a fast acoustic material and when deposited on silicon the combination is referred to as "fast on slow". The switch to ScAlN and the presence of SiO₂ makes the acoustic velocity interplay complex and can be referred to as "fast-slow-fast".

Figure 6.5 shows that higher surface acoustic modes exist for wavelength 1,000 nm up to around 16 GHz. They are most likely all higher Rayleigh modes as opposed to shear horizontal waves modes, despite the complex velocity structure (fast thin-film on slow substrate) of the substrate, similar to those found in [72]. The fourth mode can be the fourth harmonic of the fundamental mode, however, double-finger IDTs are known to suppress even-harmonic overtones in favor of odd-harmonic ones due to the finger electrode placement [7]. Alternatively, while Love modes are generally found in plate structures, they have higher frequencies than Rayleigh waves due to their strong shear components and may be a possible explanation as well [75].

A closer look at the wide frequency modes generated within the delay-lines is shown in Figure 6.6 for $\lambda = 1,000$ nm. These modes differ from surface modes in their wide high-frequency characteristic and thus have a bulk component. Modes marked B1 and B3 have a FWHM of almost 0.3 GHz, yet still have a peak shape in the frequency domain, making them possibly a pseudo-SAW (surface skimming or leaky SAW) [7, 75–77]. The "fast on slow" material combination seems more prone to supporting spurious modes, including acoustic waves with BAW components [75]. This is unlike in Chapter 3 where

Figure 6.5: An overview of SAW resonances from the $\lambda = 1,000\text{ nm}$ delay-line shown in Figure 6.3. An overview of resonances excited by the delay-line into higher frequencies, however, the nature of the waves is unclear. The resonances above 10 GHz display an unusual, peak and dip, characteristic in the the transmission. It may be possible that these are leaky SAW waves.

Figure 6.6: An overview of BAW resonances from the $\lambda = 1,000\text{ nm}$ delay-line shown in Figure 6.3. This delay-line also displayed wide frequency resonances which are most likely bulk acoustic waves. Transmissions were time-gated for clarity.

the ZnO/Si multilayer was a "slow on fast" material combination and no bulk modes were observed.

6.3.2 100 nm ScAlN

The thinner, 100 nm, ScAlN substrate delay-line scattering parameters can be seen in Figure 6.7. In the upper panel, the reflection S_{11} shows two modes for the first three wavelengths, however, as compared to the thicker 300 nm sample, the second mode is not more pronounced than the fundamental one. In the lower panel, the transmission S_{21} tells a similar story, as the fundamental mode is present for the larger two wavelengths, whereas there was no easily discernible transmission of the fundamental mode for the thicker sample. The reason can be the complex interplay of the thin-film thicknesses. As the fast ScAlN gets thinner more of the SAW piezoelectric and strain wave can penetrate into the single-crystalline silicon substrate. This in turn equalizes the coupling of the two modes to the substrate as there is less of a waveguiding effect for the higher-order mode.

The time-domain for the second mode in Figure 6.8 is quite similar to the thicker sample as well. The two separate components of the wave are present, but differently, both are visible for all wavelengths. The TTE is seen only for $\lambda = 800$ nm, as opposed to the $\lambda = 1,000$ nm for thicker sample and can be a measurement artifact.

For both ScAlN thicknesses, a more closer look at the time-domain for the fundamental mode R1 is given in Figure 6.9. The SAW transmissions are larger for the thinner sample for both wavelengths, which corresponds to the resonances seen in Fig. 6.7. The thicker ScAlN sample has a second peak following the first, which is most likely a spurious transverse wave similar to the one seen for the R2 mode in Fig. 6.4. Why it is only present for the thicker sample is unclear, but the ScAlN layer thickness origin is a likely cause as more of the SAW is confined in the faster ScAlN.

6.4 OVERVIEW OF SAW CHARACTERISTICS

The extracted SAW velocities v_{SAW} of modes R1 and R2 for both samples are shown in top part of Figure 6.10. Mode R1 has a velocity around $\sim 4,000 \text{ m s}^{-1}$ for both ScAlN thicknesses. The velocity increases more visibly for the thinner ScAlN with increasing wavelength, which parallels more penetration into the silicon substrate. The low velocity compared to the SAW velocity in silicon indicates that the SiO_2 also plays a large role in the overall velocity of SAWs in this structure. The piezoelectric fields accompanying the acoustic waves most likely concentrate in the SiO_2 layer and are in turn influenced more in their propagation [78].

Figure 6.7: Vector network analysis of NIL delay-lines on 100 nm ScAlN/100 nm SiO₂/Si. The delay-lines show both R1 and R2 modes more clearly, as opposed to the thicker films. The transmission also shows the additional wide frequency peaks after the R2 mode.

Figure 6.8: Time-domain of VNA S_{21} shown in Figure 6.7. Seen are the times of arrival of SAWs on the receiving IDTs in S_{21} . Similarly as in Figure 6.4, the arrival time for all wavelengths is around $t \approx 200$ ns. For the wavelength $\lambda = 800$ nm (seen in yellow), the triple reflection is at $t \approx 600$ ns. The double lobed feature of the detected SAW (second lobe at $t \approx 300$ ns) can be from a spurious acoustic mode.

Figure 6.9: Time-domain of R1 mode for both ScAlN thicknesses. Seen are the times of arrival of SAWs on the receiving IDTs in S_{21} . Similarly as in Figure 6.4, the arrival time for all wavelengths is around $t \approx 200$ ns. For the wavelength $\lambda = 800$ nm (seen in yellow), the triple reflection is at $t \approx 600$ ns. The double lobed feature of the detected SAW (second lobe at $t \approx 300$ ns) can be from a spurious acoustic mode.

The lower part of Figure 6.10 shows the experimental electromechanical coupling coefficient k_{eff}^2 for delay-lines on both ScAlN samples obtained using Ref. [10]. The 100 nm ScAlN delay-lines have a low coupling, around $\sim 0.5\%$, for both modes, which is consistent with their low power in VNA measurements. A thin piezoelectric film, in conjunction with a thin SiO_2 layer, most likely both contribute to the low k_{exp}^2 values [76, 79].

The delay-lines on the thicker ScAlN thin-film have a larger electromechanical coupling, but with a minimum close to 0.5% for $\lambda = 800$ nm. The coupling rises for mode R2 up to 2.5% for smaller wavelengths via a larger fraction of the SAW existing in the piezoelectric film. On the other hand, the resonance for $\lambda = 520$ nm is quite wide and the high coupling can also be a measurement artifact. However, the resonance of the preceding wavelength (640 nm) does not have such frequency widening and its coupling coefficient ($\sim 1.5\%$) is thus closer to the actual value.

Numerical simulations in COMSOL Multiphysics are used to attempt to investigate the unusual spurious behavior of this material structure (see Chapter 5), particularly the double wave features seen in the time-domain (Figs. 6.4 and 6.8) with regards to the strain and piezoelectric field shape of mode R2. Unfortunately, the 2D simulations (x - and z -axis) were insufficient to help explain this further as no higher-order modes were calculated to be present. The most likely cause is that both surface waves have a significant transverse shear component, which cannot be simulated in just two dimensions. Nonetheless, the fundamental Rayleigh modes were found and their calculated character-

Figure 6.10: SAW properties of delay-lines on ScAlN (300 nm & 100 nm)/SiO₂/Si. Top: SAW velocities, bottom: estimation of the effective electromechanical coupling constant K_{eff}^2 , left side: $h_{\text{ScAlN}} = 100$ nm and right side: $h_{\text{ScAlN}} = 300$ nm. Indicated are as well the two measured modes R1 and the faster R2. Clearly, a thicker ScAlN thin-film yields better SAWs. Values were taken from tables A.5 and A.6. Stars denote values obtained from numerical simulations.

istics are indicated with stars in the Figure 6.10, both for velocity and the corresponding electromechanical coupling factor. While the velocity is close to the experimental one, the calculated coupling is around 0.25 % for both ScAlN film thicknesses. This is lower than the experimental values found, but can be due to the missing transverse elements.

6.5 CONCLUSION

In this chapter, we discussed the fabrication IDT delay-lines with features down to 65 nm using nano-imprint lithography on a novel Sc-doped AlN piezoelectric thin-film on silicon with two different thicknesses, despite difficulties due to small substrate size and particle contamination. The delay-lines were characterized with a network analyzer and found to have sharp SAW resonances and with higher modes up to 16 GHz. The nature of the surface acoustic waves is unusual in the time-domain, where it was seen that the excited waves have a many mode profile attributed to transverse SAWs excited

in addition to Rayleigh waves. The velocity of the fundamental mode was lower than both the silicon and (Sc)AlN acoustic velocities and is concluded to be influenced by the presence of the thin SiO₂ layer in-between the films, in which the acoustic and piezoelectric fields concentrate. This additional layer also enables higher SAW modes with velocities close to the cut-off velocity of the silicon substrate. The presence of the fast ScAlN thin-film is also attributed as the source of the generation of wide high-frequency bulk acoustic modes seen in the transmission S_{21} of the network analysis. 2D numerical simulations were unfortunately insufficient to explain the presence of higher and spurious modes and waves seen in the experiments. The novel material clearly performs well with surface acoustic devices, however, further theoretical and numerical work is needed to fully explain its characteristics and interplay with other thin-films on silicon substrates.

LESSONS AND NEXT STEPS FOR NOVEL ACT DEVICES

In this chapter, we present the application of lessons from previous chapters into designing and implementing novel acoustic devices. The focus will not only be on enhancing IDT efficiency for SAW generation, but also to combine acoustic devices via SAW resonators with quantum electronic experiments on silicon in the exciting new field of silicon quantum acoustics, a phonon analogue to quantum optics on a chip [6, 32, 80].

In the first section we look at the details of fabrication and processing. This is followed by an IDT redesign section. Next, we look at piezoelectric materials and their implementation into the novel fabrication and IDT designs. And lastly, we present considerations when introducing resonators into the whole process.

7.1 RETHINKING FABRICATION

Any processing has the potential to damage thin-films, via chemical or mechanical interactions. This is seen in Chapter 2 and 3, where ZnO thin-film imperfections were made more severe via fabrication steps post-deposition (see Fig. 2.2). The morphological structure of the thin-films turned out to be sensitive when exposed to the varying temperatures necessary in the RIE step of nano-imprint lithography. Further, imprint pattern transfer was degraded in quality via particle contaminates from repeated substrate exposure to environments outside of or in less-than-ideal cleanroom conditions 6.1. While cleaning in acetone/IPA/DI water ultrasonic procedures alleviated most of the particle contamination, the thin-films themselves may have been affected mechanically.

7.1.1 The optimized process flow

The proposed remedy in processing is simple, NIL should be implemented as early as possible in the fabrication. The most obvious time for processing silicon acousto-electronic devices is after the functionalization of the silicon

Figure 7.1: Proposed structure of future acousto-electronic devices. At the heart of the change in fabrication is the move of the IDT underneath the piezo-electric material (marked in the image as *PE*). This allows the integration of silicon quantum dot devices and acoustic elements with fewer steps. When the IDTs, bragg mirror elements, and quantum dot barrier gates are fabricated in a single step, a more accurate lateral spacing and, thus device functionality, is enabled.

substrate with selective p- and n-type doping, just before one would deposit piezoelectric material. This has the added advantage of keeping the necessary surface clean as most of the processing steps are standard silicon processing and can be done in-house (such as at the University of Twente NanoLab). Even if the doping steps have to be outsourced, rigorous cleaning processes can be used since the wafers do not have the sensitive piezoelectric layers yet.

After NIL, any additional steps, such as capping with atomic layer deposition (ALD) and e-beam lithography (EBL) definition of further metallic leads, gates or structures, can proceed without the disadvantages a piezoelectric layer brings, e.g.: contaminated surface or electron back-scattering during EBL, as the substrate is still only a silicon platform. In our fabrication, after NIL, we have cut the silicon wafer into small, sample sized pieces, but NIL can be alternatively processed wholly on wafer scale, even RIE etching and metallization. An example of the proposed sample structure using this process flow is seen in fig 7.1.

The downside of processing NIL and other metallic structures on silicon first, is that noble metals have to be used due to the high temperatures in further processing steps, namely ALD or piezoelectric deposition. And while giving up wafer scale processing after NIL may seem like a big disadvantage, small sample sizes are useful as many experimental deposition instruments are limited in sample substrate size.

7.1.2 Better capping material

A closer look at the negative effect of very thin sputtered material on SAW propagation was given in Chapter 4. While propagation loss due to 20 nm SiO_2 was shown to be not too excessive in LiNbO_3 in Fig. 4.4, only an additional $\sim 3 \text{ dB mm}^{-1}$, complicated substrates with many layers (e.g.: as seen in Ch. 2 and 3) can exhibit higher loss or even no transmission signal as seen in Fig. 3.8. Propagation loss increases with frequency (as seen in Fig. 4.5 and a good reference [44]) and additional surface structures, such as metallic gates, only provide more scattering sources for propagating SAWs (e.g.: as seen in Ch. 2), making surface material quality a high priority.

Sputtered SiO_2 is mostly deposited as SiO_x and can be quite electrically leaky when not optimized for specific applications [81]. ALD Al_2O_3 is more advantageous as it is conformal, uniform, and complimentary to both silicon quantum devices and acoustic applications [82, 83]. Thus, it can be used as both a capping and protection layer on all types of metallic structures prior to piezoelectric material deposition. The disadvantage of ALD alumina is the resulting uneven surface in the area of the IDTs and other fabricated structures, which can have a deleterious effect on piezoelectric material growth during deposition and the finished sample surface roughness [46].

7.2 ALTERNATIVE IDT DESIGNS FOR PROPAGATING HIGH-FREQUENCY SAWs

7.2.1 Impedance matching

Improper impedance matching of IDTs to the peripheral circuit (50Ω) can result in poor SAW generation, reflective behavior of SAWs within the IDT, and also resonator behavior in the propagation area next to the IDT, as seen on LiNbO_3 in Chapter 4. Impedance matching for better IDT performance is thus crucial for better device performance. One of the methods is through numerical simulation as seen in Chapter 5, resulting in a clearer picture of the ideal IDT sizes and lengths (see tables in Appendix B).

Further, the simulated structure needs to take into account the metal electrodes and the resulting shape of the thin-films on the surface [46]. This is true especially for higher modes, which are more advantageous for ACT, but in turn more sensitive to surface defects [33]. An example of such a simulated structure along with the resulting impedance characteristics is shown in Figure 7.2.

Additionally, the IDT bus bars and leads to contact pads need to be impedance matched as well. One need not use numerical simulation, but a quick and "back-of-the-envelope" calculation of high-frequency waveguide matching can be found with online electrical engineering calculators.

Figure 7.2: IDT material structure and resulting impedance matching conditions. a) device substrate underneath IDT used in numerical simulations. Substrate morphology is due to thin ALD Al_2O_3 layers (light blue) which are conformal on the buried electrodes (purple), making the ZnO and capping layers (dark red and yellow) have a step like shape. b) The calculated IDT electromechanical coupling coefficient for several ZnO thicknesses, for a wavelength $\lambda = 260$ nm. c) The calculated IDT finger pair numbers for impedance matching to 50Ω based on the size of the IDT aperture using the model in Chapter 5 for $\lambda = 260$ nm.

7.2.2 Acoustic reflection and transverse mode minimization

For thin-films (ca. < 100 nm), small wavelengths ($\lambda \sim h_{\text{layer}}$), and strong piezoelectric substrates (LiNbO_3) the SAW reflection of any surface defect is quite strong and leads to resonant behavior (seen in LiNbO_3 and indicated in Figure 5.10). One way to limit this effect is to design IDTs with gradually decreasing feature size, thus, decreasing the IDT metallization ratio at the edges. The metallization ratio is the finger size to spacing ratio in one wavelength of an IDT (see IDT capacitance C_S in Ch. 5 for more details). This can help couple the propagating SAW from the IDT into the free surface [7]. An example is shown in Figure C.4b.

Dummy fingers extending from the opposing electrode suppress the generation of transverse shear waves within the IDT. The spacing from finger end to dummy electrode should be smaller than the target wavelength.

Additionally, SAW reflect on the edge of the IDT before exiting into the propagation region. To minimize this effect, single-finger IDTs should have an extra finger ($N + 1/2$ number of finger pairs) and double-finger IDTs should split one double-finger to the edges of the IDT.

And finally, one design consideration for propagating SAW type devices is to limit the length of the receiving IDT. This will limit the back-reflection of the SAW and decrease transit echos within the free propagation and active device area.

Figure 7.3: IDT designs for higher harmonics generation. a) A 5-2 split IDT has an extra floating electrode and is capable of exciting the first four harmonics of the fundamental Rayleigh mode [63]. b) An IDT with a 90 % metallization ratio, capable of generating up to the 11th harmonic [84].

7.2.3 High harmonics not modes for high-frequency SAWs

While higher modes give access to higher frequency acoustic waves, they require a specific thin-film material and thickness combination, which may not be achievable at very small wavelengths (see Chapter 5). Even more, modes higher than the Sezawa (first higher-order) mode have a smaller electromechanical coupling to the substrate and thus, may not be strong enough for high-frequency applications (as seen e.g. in Chapter 2). Further, in "fast on slow" substrates the fundamental mode is most efficient, higher modes having a bulk component which can have adverse affects on device performance.

Generating higher harmonics of the fundamental Rayleigh mode is an interesting alternative to higher modes for high-frequency SAW devices. IDTs designed to excite higher harmonics involve either a specific combination of finger widths, placement order or increase of the metallization ratio of the IDT, similar to unidirectional IDTs [7, 63, 84, 85]. An example of both can be seen in Figure 7.3.

Unfortunately, larger IDT feature sizes and longer periodicity of the IDT single cell, can place a lower limit on the IDT wavelength or can make impedance matched IDT too long for the sample.

7.3 PIEZOELECTRIC MATERIAL CONSIDERATIONS

7.3.1 material quality requirements

The ideal thin-film piezoelectric material has small grains (much smaller than wavelength), which are densely packed with a small surface roughness, and very few defects, such as embedded particulates or pin holes (see Chapter 3). Succinctly put, the material should be optimized for the specific thickness and function. Likewise, a dedicated tool for deposition would be ideal for quality control and a purging and cleaning step of the tool before deposition if, for example, going from oxides to nitrides, is needed.

If the process flow of the previous section 7.1 is followed, piezoelectric material may even be deposited outside of the cleanroom as the last steps do not require any lithography smaller than 1 μm . Experimental material deposited outside a cleanroom can be interesting for novel applications, however, this would be at a cost to some device functionality as particles will be embedded inside the film.

7.3.2 Novel materials and other techniques

There are two routes to achieve high-frequency acoustic waves for acousto-electronic devices: fast material ($>5,000\text{ m/s}$) or a clever material combination for higher acoustic wave modes. Having only a single piezoelectric layer can simplify fabrication, however, in a *fast on slow* material configuration (AlN on Si) spurious and bulk modes can complicate the acoustic experiments. AlN and Sc-doped AlN have been the focus of investigation for fast and highly efficient SAW generation, but on fast substrates like diamond (in the slow on fast configuration) [73, 86].

Alternatively, single-crystal materials have recently been integrated with functionalized silicon [87]. Here, LiNbO_3 was bonded onto a silicon wafer using an ion-cutting process leaving behind only a thin-film. This method is complimentary to the process flow outlined in the previous sections, as the piezoelectric is added last, but can put a lower limit on the SAW wavelength depending on the thickness of the residual LiNbO_3 film.

Lastly, while the sol-gel derived ZnO thin-film did not function as expected in Chapter 3, chemically synthesized piezoelectric thin-films, even organic ones, are currently being developed, although their performance at high frequencies is limited [88].

The purpose of this section was not to lose the reader in a sea of choices, but rather to motivate the new acoustic scientist with potential alternative piezoelectric material sources. Using the process flow outlined above, there is much flexibility in the choice and character of deposition of the material,

allowing a comparison of materials and methods for various applications on silicon. However, we caution that optimization of the chosen material for a specific acousto-electronic device structure and functionality is still very much needed.

7.4 SAW RESONATOR DESIGN FOR SI QUANTUM DOTS

In this section we apply the know-how of the previous sections, and indeed the entire thesis, to design silicon quantum acoustic devices. In principle, such devices combine a quantum dot device and a phonon source, such as an IDT or even a surface acoustic wave resonator. These surface acoustic wave devices were first tested on GaAs, the bedrock of acousto-electronic experiments, where quantum dot tunneling was tuned by phonon pumping from nearby IDTs [89, 90], with a standing wave in a resonator [2, 91], or even enabling transfer of electrons between two distant quantum dots [21].

Here, we will focus on designing a silicon quantum dot device which will be influenced with standing waves via a surface acoustic wave resonator.

7.4.1 Cavity conditions

A surface acoustic wave resonator is like any other resonating device, comprised of a cavity, surrounded by full or permeable mirrors, and a driving source which pumps the cavity with, in this case, SAWs.

The surface acoustic cavity can be trivially large, but only in so far as it fulfills the cavity condition $l_{cavity} = N * \lambda/2$, where N is an odd positive integer. This condition assumes one very important point, that the surface acoustic wave is mostly reflected from the edge of the mirror, so called *edge reflection*. This is true for (i) piezoelectric materials with low electromechanical coupling, (ii) single-crystal substrates like LiNbO₃, (iii) very thin piezoelectric films and (iv) small SAW wavelengths, where any surface discontinuity greatly reflects and diffracts the traveling SAW [7, 9].

We come to the next logical question, how does one make a mirror for a surface acoustic wave? The careful reader can already guess that it has something to do with discontinuities on the surface and that is correct and for our purpose a SAW mirror is a grating made of IDT finger element of $\lambda/4$ width with a period of $\lambda/2$ which is called a Bragg mirror. This grating can consist of metallic fingers, shorted or floating, or even grooves within the substrate. In edge reflection, the traveling SAW is slightly reflected back at the edge of each grating element slowly adding up to total reflection. If one is not in the edge reflection mode, the reflection is taken to be the middle of the grating element. The latter case also modifies the cavity condition by the

Figure 7.4: IDT resonator schematics for quantum acoustic devices. a) A resonator with IDTs inside the cavity. One IDT is shorter to act as a receiver. b) A resonator with a IDTs outside the cavity. The phonon cavities have a sketch of a double quantum dot defined by barrier gates and a lead gate in orange. The positioning of the IDTs, the mirrors and even the QDs with respect to one another is very important.

addition of a grating element length ($\lambda/4$), twice the distance to the middle of the element at each of the cavity.

Each grating element has a reflectivity and one can calculate how many elements are needed for full reflection or the distance the SAW penetrates into the mirror. A very good practical example is given in [56].

7.4.2 IDT-mirror spacing

The cavity driver, the IDT, needs to be carefully positioned with respect to the mirror elements for efficient SAW reflection. There are two configurations of IDTs, mirrors and the cavity itself (see Fig. 7.4). The first, the IDTs are inside the cavity which is made by long Bragg mirrors on the outside. And the second, the IDTs are outside the cavity, which is made by two semi-permeable short Bragg mirrors or one short and one long one.

In the first case, care should be taken that the SAW reflects efficiently from the mirrors, but also forms a standing wave in the cavity. In the one port resonator, the cavity forms between the IDT and one or both mirrors, or

Figure 7.5: IDT-mirror distance for cavity formation. a) An IDT and mirror separation $d_1 = N * \lambda/2 + \lambda/8$. The distance is set so that a SAW traveling from the IDT has a node on the edge of the mirror, enabling high SAW reflection to form a cavity. b) An IDT and mirror separation $d_2 = N * \lambda/2 + 3\lambda/8$ has a low SAW reflectivity as the traveling SAW has an anti-node (peak) on the edge of the mirror.

indeed over the whole cavity between mirrors. In the two port resonator, the cavity can be placed between two IDTs in-between the mirrors, just between one IDT and a mirror, or extending the whole length between the mirrors. Many variations exist, so too for the second case of IDTs outside the Bragg mirrors.

Assuming edge reflection, the separation condition for good SAW reflection between mirror-IDT in order to form a cavity is $N * \lambda/2 + \lambda/8$, where N is an odd integer. This places the edge of the mirror on the node of the SAW generated by the IDT (Fig. 7.5a). If the opposite were to be desired, that no cavity form between mirror and IDT, then the condition is amended to $N * \lambda/2 + 3\lambda/8$. This is so that, if a standing wave is generated from an IDT, its node elements would (not) coincide on the edge of the mirror element (Fig. 7.5b). One would use the former condition for IDTs placed inside a cavity and the latter for IDTs outside a cavity. A sketch of the two different resonator designs is shown in Figure 7.4. An excellent overview of cavities and resonator is given by [9], for behavior of two port resonators see [92], and for an experimental an experimental analysis to edge reflection and IDT-mirror distance placement see [67, 93].

7.5 CONCLUSION

We have presented a roadmap to a future silicon quantum acousto-electronics platform for novel applications in the field of quantum acoustics. This chapter gives an impression of the scale of thinking, care and work that goes into even a single device. From background and simulations, to fabrication and material,

and finally to function. This represents a multi-faceted problem which, in many cases, can only be optimized experimentally. Nonetheless, a viable path forward has been shown.

And finally, an overview of a new nano-imprint template can be found in Appendix C. Many of the principles for acoustic devices mentioned in this outlook have been implemented into the design and an example is shown in Figures C.3 and C.4.

DETAILS OF EXPERIMENTAL SAW DEVICES

A.1 ZnO/SiO₂/SI MULTILAYER THIN-FILMS

Table A.1: SAW delay-line resonance frequencies, velocities, and estimation of the effective electromechanical coupling constant K_{eff}^2 . Experimental and sample specific values found for R1, R2, and in some cases, SAW R3 modes. Some resulting velocities and K_{eff}^2 values are too high for R3 modes (indicated with *), suggesting a non trivial situation, *e.g.*: leaky SAWs, SAW is actually a BAW, or the measurement was faulty.

λ [nm]	R1			R2			R3		
	f [GHz]	v [m s ⁻¹]	K_{eff}^2	f [GHz]	v [m s ⁻¹]	K_{eff}^2	f [GHz]	v [m s ⁻¹]	K_{eff}^2
1000	3.59	3588	0.019	5.37	5373	0.018	7.96	7956	0.012
800	4.15	3320	0.015	6.44	5150	0.016	—	—	—
640	4.79	3064	0.012	7.79	4988	0.018	—	—	—
520	5.44	2829	0.018	—	—	—	—	—	—
500	4.47	2233	0.011	8.26	4130	0.033	10.55	5275	0.026
400	5.16	2062	0.014	9.58	3832	0.036	12.40	4960	—
320	6.14	1963	0.016	11.40	3646	0.022	—	—	—
260	—	—	—	12.77	3320	0.042	—	—	—

Table A.2: SAW delay-line material and IDT characteristics. The ZnO thickness is $h_{\text{ZnO}} = 100$ nm, the electrode thickness $h_{\text{el}} \approx 40$ nm and the mean grain size for sputtering (DF IDTs) is $\bar{D} = 37.91$ nm and for PLD (SF IDTs) is $\bar{D} = 18.57$ nm (from Table 3.2).

λ [nm]	h_{ZnO}/λ	h_{el}/λ	$\lambda/\bar{D}$
1000	0.10	0.04	26
800	0.13	0.05	21
640	0.16	0.06	17
520	0.19	0.08	14
500	0.20	0.08	27
400	0.25	0.10	22
320	0.31	0.13	17
260	0.38	0.15	14

A.2 LITHIUM NIOBATE SUBSTRATES

Table A.3: SAW delay-lines on LiNbO₃. Resonance frequencies, velocities, estimation of the effective electromechanical coupling constant K_{eff}^2 , period of resonant oscillations Δf and the corresponding cavity size L . There appears to be a trend of lower velocity, lower K_{eff}^2 . Period Δf is holding constant, while the cavity shrinks. A likely scenario is that as the wavelength shortens, the impedance mismatch of the IDT gets higher making the active region of the IDT shorter.

λ [nm]	f [GHz]	v [m s ⁻¹]	K_{eff}^2	Δf [MHz]	L [μm]
1000	3.64	3635	0.001	3	333
800	4.53	3621	0.023	3	267
640	5.63	3604	0.008	3	213
520	6.89	3583	0.012	3	173
500	7.83	3917	0.071	—	—
400	9.70	3882	0.024	—	—
320	12.14	3885	0.040	—	—
260	14.51	3773	0.015	—	—

Table A.4: SAW delay-lines on LiNbO₃ with a 20 nm SiO₂ capping layer. Resonance frequencies, velocities, and estimation of the effective electromechanical coupling constant K_{eff}^2 . Experimental and sample specific values found for R1 and R2 SAW modes.

λ [nm]	R1			R2		
	f [GHz]	v [m s ⁻¹]	K_{eff}^2	f [GHz]	v [m s ⁻¹]	K_{eff}^2
1000	3.62	3623	0.009	7.25	7247	0.015
800	4.50	3603	0.013	8.92	7138	0.049
640	5.59	3575	0.011	10.88	6960	0.037
520	6.81	3541	0.005	12.75	6632	0.008

A.3 SCALN THIN-FILMS

Table A.5: SAW properties of delay-lines on ScAlN (300 nm)/SiO₂/Si. Wavelengths, resonance frequencies, velocities, and estimation of the effective electromechanical coupling constant k_{eff}^2 . Experimental and sample specific values found for R1 and R2 SAW modes.

λ [nm]	R1			R2		
	f [GHz]	v [m s ⁻¹]	K_{eff}^2	f [GHz]	v [m s ⁻¹]	K_{eff}^2
1000	4.03	4028	0.007	5.78	5775	0.012
800	4.99	3989	0.005	7.11	5691	0.006
640	—	—	—	8.67	5550	0.011
520	—	—	—	10.22	5318	0.025

Table A.6: SAW properties of delay-lines on ScAlN (100 nm)/SiO₂/Si. Wavelengths, resonance frequencies, velocities, and estimation of the effective electromechanical coupling constant k_{eff}^2 . Experimental and sample specific values found for R1 and R2 SAW modes.

λ [nm]	R1			R2		
	f [GHz]	v [m s ⁻¹]	K_{eff}^2	f [GHz]	v [m s ⁻¹]	K_{eff}^2
1000	4.21	4216	0.005	5.83	5825	0.005
800	4.98	3980	0.004	7.26	5804	0.004
640	5.81	3715	0.005	8.94	5719	0.004
520	—	—	—	10.79	5614	0.005

NUMERICAL SIMULATION INPUTS, CALCULATIONS AND RESULTS

B.1 MATERIAL CONSTANTS AND PROPERTIES

Table B.1: Material constants used in numerical simulations; density ρ , elastic stiffness coefficients c_{ij} , piezoelectric coefficients e_{ij} , relative permittivity ϵ_r and temperature coefficient of frequency TCF of ZnO, Si, SiO₂, Al, and non-rotated LiNbO₃.

Material		Si ⁺²	SiO ₂ ⁺¹	ZnO ⁺¹	Al ⁺³	LiNbO ₃ ⁺⁴
Density (kg m ⁻³)	ρ	2330	2350	5665	2700	4628
Elastic constants (Pa $\times 10^{11}$)	C_{11}	1.657	0.785	2.0900	1.11	1.9839
	C_{12}	0.639	0.161	1.2035	0.61	0.5472
	C_{13}	0.639	0.161	1.0460	0.61	0.6513
	C_{14}	-	-	-	-	0.0788
	C_{33}	1.657	0.785	1.6570	1.11	2.279
	C_{44}	0.796	0.312	0.4230	0.28	0.5965
	C_{66}	0.796	0.312	0.4440	0.28	0.73
Piezoelectric constants (C m ⁻¹)	e_{15}	-	-	-0.480	-	3.69
	e_{22}	-	-	-	-	2.42
	e_{31}	-	-	-0.573	-	0.3
	e_{33}	-	-	1.321	-	1.77
Relative permittivity	ϵ_{11}	11.68	2.37	7.38	1	45.6
	ϵ_{33}	11.68	2.37	9.05 ⁺⁵	1	26.3
Temp. coef. of frequency (ppm/°C)	TCF	-33 ⁺⁶	-85 ⁺⁷	34 ⁺⁷	-	-75 ⁺⁸

⁺¹ from [28]; ⁺² from [94]; ⁺³ from [95]; ⁺⁴ from [96];

⁺⁵ from [60]; ⁺⁶ from [97]; ⁺⁷ from [40]; ⁺⁸ from [98];

Table B.2: Material constants used in numerical simulations; density ρ , elastic stiffness coefficients c_{ij} , piezoelectric coefficients e_{ij} , relative permittivity ϵ_r and temperature coefficient of frequency TCF of Si, SiO₂, AlN and estimated for Sc_{0.26}Al_{0.74}N.

Material		Si ⁺²	SiO ₂ ⁺¹	AlN ⁺⁹	Sc _{0.26} Al _{0.74} N ⁺¹⁰
Density (kg m ⁻³)	ρ	2330	2350	3230	3560
Elastic constants (Pa $\times 10^{11}$)	C_{11}	1.657	0.7850	4.1	3.2
	C_{12}	0.639	0.1610	1.49	1.35
	C_{13}	0.639	0.1610	0.99	1.15
	C_{14}	-	-	-	-
	C_{33}	1.657	0.7850	3.89	2.4
	C_{44}	0.796	0.3120	1.25	0.98
	C_{66}	0.796	0.3120	1.305	0.925
Piezoelectric constants (C m ⁻¹)	e_{15}	-	-	-0.480	-0.33
	e_{22}	-	-	-	-
	e_{31}	-	-	-0.58	-0.72
	e_{33}	-	-	1.55	2.33
Relative permittivity	ϵ_{11}	11.68	2.37	8	13.06
	ϵ_{33}	11.68	2.37	9.5	13.06
Temp. coef. of frequency (ppm/°C)	TCF	-33 ⁺⁶	-85 ⁺⁷	-27.2 ⁺¹¹	-27.2 ⁺¹¹

⁺¹ from [28]; ⁺² from [94]; ⁺⁶ from [97]; ⁺⁷ from [40];

⁺⁹ from [99]; ⁺¹⁰ from [100]; ⁺¹¹ from [101];

Table B.3: Material acoustic wave velocities. The velocities of acoustic waves for materials used in this thesis, where v_{SAW} is the surface acoustic wave velocity in bulk material, $v_l = \sqrt{C_{11}/\rho}$ the bulk longitudinal velocity and $v_t = \sqrt{C_{44}/\rho}$ the bulk transverse velocity. All values are calculated using parameters from tables in this Appendix.

material	v_{SAW}^{*1} [m s ⁻¹]	v_l [m s ⁻¹]	v_t [m s ⁻¹]
AlN (002)	5800	11266	6220
Sc _{0.26} Al _{0.74} N	4765	9480	5246
ZnO (002)	2650	6073	2730
SiO ₂	3300	5779	3643
Si	5083	8433	5844

*1 calculated using COMSOL Multiphysics.

B.2 NUMERICAL SIMULATION AND IDT MODEL RESULTS

Table B.4: Parameters calculated from equation (5.2) and (5.5) for the R1 and R2 SAW mode in a ZnO (100 nm)/Si multilayer. λ is the IDT wavelength, N_{stamp} is the number of finger pairs currently in the NIL stamp design, K_{sim}^2 is the calculated electromechanical coupling constant, Z_0 is the impedance at resonance, and N_{match} is the ideal number of finger pairs to achieve a match to $Z = 50 \Omega$.

IDT		R1			R2		
λ [nm]	N_{stamp}	K_{sim}^2 [%]	Z_0^{sim} [Ω]	N_{match}	K_{sim}^2 [%]	Z_0^{sim} [Ω]	N_{match}
260	1346	0.3	1	181	2.7	0.1	50
320	1092	0.4	1	183	2.9	0.1	55
400	876	0.5	2	199	2.6	0.2	56
500	700	0.4	4	171	2.3	0.5	66
520	673	0.4	3	171	2.3	0.4	57
640	546	0.5	4	162	2.7	0.5	55
800	438	0.3	13	219	1.7	1.6	77
1000	350	0.4	17	200	1.6	2.9	83

Table B.5: Parameters calculated from equation (5.2) and (5.5) for the SAW R1 mode in LiNbO₃. λ is the IDT wavelength, N_{stamp} is the number of finger pairs currently in the NIL stamp design, K_{sim}^2 is the calculated electromechanical coupling constant, Z_0 is the impedance at resonance, and N_{match} is the ideal number of finger pairs to achieve a match to $Z = 50 \Omega$.

IDT		bare LiNbO ₃			SiO ₂ /LiNbO ₃		
λ [nm]	N_{stamp}	K_{sim}^2 [%]	Z_0^{sim} [m Ω]	N_{match}	K_{sim}^2 [%]	Z_0^{sim} [m Ω]	N_{match}
260	1346	8.1	3	10	1.0	22	29
320	1092	7.7	5	11	1.1	34	29
400	876	7.4	10	13	1.3	55	29
500	700	7.1	21	14	1.5	92	30
520	673	6.5	17	12	1.6	72	25
640	546	6.4	33	14	1.8	117	26
800	438	6.6	62	15	2.0	200	28
1000	350	6.4	124	17	2.3	347	29

B.3 EXPERIMENTAL IDT PERFORMANCE FROM S_{11}

Table B.6: IDT performance extracted from S_{11} for the R1 and R2 SAW mode in a ZnO (100 nm)/Si multilayer. λ is the IDT wavelength, f_0 is the resonance frequency, K_{exp}^2 is the experimental electromechanical coupling constant, R_{11} is $Re\{Z_{11}\}$, and X_{11} is $Im\{Z_{11}\}$, where Z_{11} is from S_{11} using eq. (5.8).

IDT λ [nm]	R1				R2			
	f_0	K_{exp}^2 [%]	R_{11} [Ω]	X_{11} [Ω]	f_0	K_{exp}^2 [%]	R_{11} [Ω]	X_{11} [Ω]
1000	3.59	1.9	22	-21	5.37	1.8	23	-1
800	4.15	1.5	28	-10	6.44	1.6	31	10
640	4.79	1.2	22	-13	7.79	1.8	25	16
520	5.44	1.8	31	5	-	-	-	-
500	4.47	1.1	36	-17	8.26	3.3	30	-12
400	5.16	1.4	33	-16	9.58	3.6	29	-12
320	6.14	1.6	29	-11	11.40	2.2	27	-8
260	-	-	-	-	12.77	4.2	22	-7

Table B.7: IDT performance extracted from S_{11} for SAWs on LiNbO₃. λ is the IDT wavelength, f_0 is the resonance frequency, K_{exp}^2 is the experimental electromechanical coupling constant, R_{11} is $Re\{Z_{11}\}$, and X_{11} is $Im\{Z_{11}\}$, where Z_{11} is from S_{11} using eq. (5.8).

IDT λ [nm]	R1			
	f_0	K_{exp}^2 [%]	R_{11} [Ω]	X_{11} [Ω]
1000	3.64	0.1	15	34
800	4.53	1.9	84	0.6
640	5.63	0.6	118	-48
520	6.89	1.0	28	-31
500	7.83	5.8	24	-10
400	9.70	2.0	43	0.1
320	12.14	3.3	39	-30
260	14.51	1.2	38	25

Table B.8: IDT performance extracted from S_{11} for SAWs on SiO₂ capped LiNbO₃. λ is the wavelength of the IDT, f_0 is the resonance frequency, K_{exp}^2 is the experimental electromechanical coupling constant, R_{11} is $Re\{Z_{11}\}$, and X_{11} is $Im\{Z_{11}\}$, where Z_{11} is from S_{11} using eq. (5.8).

IDT λ [nm]	R1				R2			
	f_0	K_{exp}^2 [%]	R_{11} [Ω]	X_{11} [Ω]	f_0	K_{exp}^2 [%]	R_{11} [Ω]	X_{11} [Ω]
1000	3.62	0.7	19	31	7.25	1.3	16	-22
800	4.50	1.0	65	51	8.92	<0.1	26	24
640	5.59	0.9	122	-49	10.88	3.0	128	-25
520	6.81	0.4	30	-32	12.75	0.6	25	-20

NEW NIL TEMPLATE FOR NOVEL ACT DEVICES

C.1 NEW NIL TEMPLATE DESIGN

Figure C.1: Design of new NIL template for SAWtrain consortium.

The NIL pattern was designed with AutoCAD software, Autodesk, Inc. The quartz template was manufactured at IMS Chips, Stuttgart. The design pattern is etched into the quartz to a depth ca. 50 – 80 nm in a negative, mirrored image. The size of the quartz template is 65 mm $\times$ 65 mm $\times$ 6.35 mm with an elevated mesa ($\sim$ 15 μ m) containing the etched design pattern.

The pattern was designed within the SAWtrain consortium, an MSCA ITN Horizon 2020 project, in collaboration with PDI Berlin, Chalmers University of Technology, Universidad Politécnica de Madrid, University of Valencia, and Nanotechnology & Devices, Germany.

Table C.1: Some NIL template parameters.

Parameter	details
pattern size	16 $\times$ 16 mm
number of IDTs	404
number of devices	224
resonators	166
delay lines	58
smallest feature size	40 nm experimental 50 nm standard
largest feature size	1 μ m
design layers	41
design objects	416,876

C.2 EXAMPLE OF DEVICES

Figure C.2: Center alignment features in NIL template with SAWtrain consortium logos.

Figure C.3: Examples of devices on NIL template a) IDT resonator with mirrors on the outside and barrier gates for quantum transport experiments (purple). Contact pads and bus-bars are shown in blue. b) An asymmetric two-port delay line. The transmitter (Tx) IDT (long orange with red on left) has $N_p = 200$, which is close to the impedance matching conditions for ZnO on Si. The receiving (Rx) IDT (short orange on right) has only 50 finger pairs for SAW reflection suppression. An ACT structure is in the delay line.

Figure C.4: Examples of devices on NIL template a) A close of the active region in the resonator shown in Fig. C.3a. b) A close up of an IDT with reduced metallization ratio fingers at the edge. Dummy fingers and bus bars are also shown.

SUMMARY

High-frequency silicon acousto-electronics are a stepping stone into a new field of research named quantum acoustics, an analogue to quantum optics on a chip. One of the main tools used in this novel field are surface acoustic waves (SAWs), which are very versatile surface strain waves used today in RF filters, gas sensors, and within quantum acoustics as phonon sources and for semiconductor band-gap modulation. It is this modulation that enables SAWs to capture and drag free carriers in what is called acousto-electronic transport (ACT).

SAWs are excited with an interdigitated transducer (IDT) on a piezoelectric substrate via the inverse piezoelectric effect. The finger width of an IDT determines the SAW wavelength and together with the substrate sound velocity, the SAW frequency. Until recently, GaAs has been the material of choice for acousto-electronic experiments because it is intrinsically piezoelectric and together with AlGaAs forms a two-dimensional electron gas (2DEG) that can be processed using well established lithographic methods. Silicon, on the other hand, is the main workhorse of the semiconductor industry and for quantum electronics research it is interesting for its long electron spin lifetimes. Unfortunately, silicon is not piezoelectric and needs additional processing in the form of piezoelectric thin-film deposition, most commonly ZnO or AlN, to be useful for ACT devices.

In this work, we explore the functionalization of silicon with ZnO thin-films for high-frequency SAW acousto-electronic transport, facilitated via small-wavelength IDTs fabricated by nano-imprint lithography. High frequencies are desirable for quantum acoustics to enter the quantum regime at low temperatures and more in general due to increasing demand in the RF industry for higher bandwidth in communication technologies.

In **chapter 2**, a photon detector is chosen as the benchmark silicon ACT device. The device is fabricated using nano-imprint lithography (NIL) defined IDTs, with feature sizes down to 65 nm, on a SiO₂ capped ZnO/SiO₂/Si multilayer system. Its function is simple in design, a laser generates excitons in the silicon substrate, which are then dragged by a traveling SAW to a biased, planar, doped-silicon diode, where they recombine and are detected as excess dark current. In practice, however, it is shown that ACT device fabrication, which involves many different environments and processes, damages the piezoelectric thin film and leads to poor transmission of SAWs along the substrate surface. Cooling the sample down to cryogenic temperatures with liquid helium does not improve the SAW transmission, nor the measured dark current at the silicon diode. A trigger and timing electrical setup is then used to lower the EM interference at the diode originating from the transmitting

IDT. Unfortunately, no dark current signal emerges from the background noise of the biased diode and we conclude that the propagating SAW is simply not strong enough to bring a detectable number of excitons to the detection diode.

A closer look at ZnO thin-films is shown in **chapter 3**. We analyze ZnO thin-films deposited on SiO₂/Si via three different methods, sputtering, pulsed-laser deposition and sol-gel spin-coating. A structural and surface properties comparison between the films is carried out using X-ray diffraction (XRD), scanning electron microscopy (SEM) and atomic force microscopy (AFM). XRD shows out-of-plane texture for all three grown thin-films to the (002) crystal direction, however, the sol-gel thin-film orientation was the poorest of the three. Surface properties differ substantially according to AFM, where the sputtered ZnO is shown to be the least rough and uneven and, thus, most suitable of the three thin-films for SAW devices. However, the SEM images of the surface reveal missing grains and pinholes within all three films. Even more, the sol-gel film is shown to be quite porous.

An acoustic characterization is carried out with vector network analysis (VNA) of NIL IDT delay lines and shows that the sputtered and PLD ZnO thin-films readily excite SAWs, while the sol-gel film is non-responsive. This likely due to its low density as compared to the other films. However, both sputtered and PLD films showed only very small SAW transmission and only for the largest SAW wavelengths. This indicates poor SAW propagation on the thin-films, likely due to the many surface defects. Wet chemical etching of the ZnO thin-film between IDTs shows only a small improvement to transmission.

An exploration of the effect a thin ~ 20 nm capping layer of sputtered SiO₂ has on high frequency SAW propagation is shown in **chapter 4**. The effect is studied on a lithium niobate (LiNbO₃) substrate, which is a single-crystal material frequently used in industry for RF SAW filters. A VNA comparison is made for four SAW wavelengths and a substantial decrease in transmission power is seen for the capped LiNbO₃ as compared to the bare one. The transmission decrease is quantified through a propagation loss analysis of delay lines with different lengths. It is shown that for the smallest wavelength of $\lambda = 520$ nm, the propagation loss increases by 3 dB for the capped substrate. The effect is shown more clearly in the time domain analysis of the SAW transmission, where a more pronounced effect is also seen in the triple transit transmission of $\lambda = 1,000$ nm.

One of the effects contributing to poor SAW performance in the previous chapters is identified as the impedance mismatch between the IDT on the substrate and the RF power source, which is matched to 50 Ω . In **chapter 5**, we numerically simulate the piezoelectric substrate used in previous chapters and apply it to an IDT equivalent circuit model for electrical impedance matching. It is found, that the IDTs used on the nano-imprint template are highly electrically and acoustically reflective due to their substantial length and corresponding high number of finger pairs. The IDT model results are compared to experimental VNA measurements in chapters 3 and 4 and the model is found to be incomplete as it does not take into account the many reflections

and resonances which occur within the fabricated devices. Nonetheless, the simulation and model are a useful tool for identifying potential IDT spurious responses and as a first approximation to minimize impedance mismatch.

The material origin of propagation loss can be mitigated by utilization of materials less susceptible to degradation during fabrication. Aluminum nitride (AlN) is a hard piezoelectric material with a high sound velocity ($\approx 10,000 \text{ m s}^{-1}$), which is attractive for access to higher frequencies without the need for small wavelengths. In **chapter 6**, a novel thin-film piezoelectric, Sc-doped AlN, is deposited on SiO_2/Si and analyzed via SAWs generated with NIL defined delay lines. The thin-film SAW generation and propagation characteristics are analyzed via a VNA and compared to the piezoelectric materials described in the previous chapters. The SAW transmissions are found to be more powerful and robust than on ZnO multilayers, however the presence of spurious shear and bulk modes may be an impediment to successful application in acousto-electronic devices.

And finally, **chapter 7** gives an outlook into a new generation of silicon ACT devices using the knowledge and experience from the previous chapters of this thesis in their design. A new thin-film material combination and fabrication process flow is proposed to minimize damage to the piezoelectric thin-films used in potential new devices. Numerical simulation and the equivalent circuit model from chapter 5 are used to assess the ideal IDT length with the proposed new material structure. Additionally, alternate IDT designs are introduced for improved generation and propagation of high frequency SAWs with larger wavelength IDTs.

SAMENVATTING

Hoogfrequente silicium akoesto-elektronica is een opstap naar een nieuw onderzoeksgebied genaamd "Quantum Acoustics" (NL: kwantumakoestiek), wat analoog is aan kwantumoptica op een chip. Eén van de belangrijkste hulpmiddelen die in dit nieuwe veld worden gebruikt zijn "surface acoustic waves" (SAWs, NL: akoestische oppervlaktegolven). Dit zijn mechanische spanningsgolven aan het oppervlak die tegenwoordig veelvuldig worden gebruikt in RF-filters, gassensoren, in de kwantumakoestiek als fononbronnen, en voor modulatie van de band gap van halfgeleiders. Deze modulatie stelt de SAWs in staat om vrije ladingsdragers vast te houden en te transporteren. Dit wordt akoesto-elektronisch transport (ACT) genoemd.

SAWs worden geëxciteerd door middel van een "interdigitated transducer" (IDT) op een piëzo-elektrisch substraat via het omgekeerde piëzo-elektrisch effect. De vingerbreedte van de IDT bepaalt de SAW-golflengte en samen met de geluidssnelheid van het substraat ook de SAW-frequentie. GaAs was tot voor kort hét materiaal bij uitstek voor akoesto-elektronische experimenten omdat het intrinsiek piëzo-elektrisch is en samen met AlGaAs een tweedimensionaal elektronengas (2DEG) vormt dat kan worden bewerkt met behulp van conventionele lithografische methoden. Silicium, daarentegen, is het belangrijkste werkpaard van de halfgeleiderindustrie en voor kwantumelektronica-onderzoek is het interessant vanwege de lange levensduur van de elektronspin. Helaas is silicium niet piëzo-elektrisch en zijn aanvullende bewerkingen nodig, in de vorm van depositie van piëzo-elektrische dunne films, meestal ZnO of AlN, om bruikbaar te zijn voor ACT-devices.

In dit werk onderzoeken we het functionaliseren van silicium met ZnO dunne-films voor hoogfrequent SAW akoesto-elektronisch transport, gefaciliteerd via IDTs met kleine golflengtes welke zijn vervaardigd met behulp van nano-imprint lithografie. Hoge frequenties zijn wenselijk voor kwantumakoestiek om het kwantumregime bij lage temperaturen te betreden en meer in het algemeen vanwege de toenemende vraag in de RF-industrie naar hogere bandbreedtes in communicatietechnologieën.

In **hoofdstuk 2** wordt een fotondetector gekozen als het maatstafgevende silicium ACT-device. Het device is vervaardigd met behulp van door nano-imprint lithografie (NIL) gedefinieerde IDTs op een ZnO/SiO₂/Si multi-laag systeem afgedekt met SiO₂. De IDTs hebben vingerbreedtes tot minimaal 65 nm. De werking heeft een eenvoudig principe. Een laser genereert excitonen in het siliciumsubstraat, die vervolgens door een bewegende SAW naar een vlakke, gedoteerde siliciumdiode worden getransporteerd. Hier recombineren ze en worden ze gedetecteerd als overtollige donkerstroom. In de praktijk, echter, wordt aangetoond dat bij de fabricage van ACT-devices, waar-

bij veel verschillende processen betrokken zijn, de piëzo-elektrische dunne-film beschadigd raakt hetgeen leidt tot een slechte transmissie van SAWs langs het substraatoppervlak. Het afkoelen van het systeem met vloeibaar helium tot cryogene temperaturen verbetert de SAW-transmissie en de gemeten donkerstroom bij de siliciumdiode niet. Een elektrische trigger- en timingopstelling wordt vervolgens gebruikt om de EM-interferentie bij de diode afkomstig van de verzendende IDT te verminderen. Helaas komt er geen donkerstroomsignaal boven de ruis van de diode uit, en we concluderen dat de zich voortplantende SAW simpelweg niet sterk genoeg is om een detecteerbaar aantal excitonen naar de detectiediode te transporteren.

In hoofdstuk **hoofdstuk 3** wordt de focus gelegd op ZnO dunne-films. We analyseren ZnO dunne-films welke zijn gedeponereerd op SiO₂/Si via drie verschillende methoden: sputteren, “pulsed laser deposition” (PLD, NL: gepulste laser depositie) en sol-gel spin-coating. Een vergelijking van de structuren oppervlakte-eigenschappen tussen de films wordt uitgevoerd met behulp van röntgendiffractie (XRD), rasterlektronenmicroscopie (SEM) en atoomkrachtmicroscopie (AFM). XRD toont uitlijning van alle drie de deponerde dunne-films aan de (002) kristalrichting, waarbij de sol-gel dunne-filmoriëntatie de slechtste was van de drie lagen. De oppervlakte-eigenschappen verschillen aanzienlijk volgens AFM, waar het gesputterde ZnO het minst ruw en ongelijkmatig blijkt te zijn en dus het meest geschikt is van de drie dunne films voor SAW-devices. De SEM-beelden van het oppervlak onthullen echter ontbrekende korrels en gaten in alle drie de dunne-films. Sterker nog, de sol-gel film blijkt behoorlijk poreus te zijn.

Een akoestische karakterisering wordt uitgevoerd met vectornetwerkanalyse (VNA) van NIL IDT-vertragslijnen en toont aan dat de gesputterde en PLD ZnO dunne-films gemakkelijk SAWs exciteren, terwijl de sol-gel dunne-film geen respons geeft. Dit komt waarschijnlijk door de lage dichtheid in vergelijking met de andere films. Zowel gesputterde als PLD dunne films vertoonden echter slechts een zeer kleine SAW-transmissie en alleen voor de hoogste SAW-golflengten. Dit duidt op een slechte voortplanting van de SAW op de dunne-films, waarschijnlijk vanwege de vele oppervlakte-defecten. Na chemisch etsen van de ZnO dunne-film tussen IDTs vertoont slechts een kleine verbetering van de transmissie.

Een verkenning van het effect dat een dunne ~ 20 nm afdeklaag van gesputterd SiO₂ heeft op hoogfrequente SAW-voortplanting wordt getoond in **hoofdstuk 4**. Het effect wordt bestudeerd op een lithiumniobaat (LiNbO₃) substraat, een monokristallijn materiaal dat veel wordt gebruikt in de industrie voor RF SAW-filters. Er wordt een VNA-vergelijking gemaakt voor vier SAW-golflengten en een substantiële afname van het transmissievermogen wordt gezien voor het afgedekte LiNbO₃ in vergelijking met het onafgedekte substraat. De transmissievermindering wordt gekwantificeerd door een analyse van het voortplantingsverlies van vertragslijnen met verschillende lengtes. Er wordt aangetoond dat voor de kleinste golflengte van $\lambda = 520$ nm het voortplantingsverlies in het afgedekte substraat toeneemt met 3 dB. Het effect wordt

duidelijker zichtbaar in de tijddomeinanalyse van de SAW-transmissie, waar een meer uitgesproken effect ook wordt gezien in de drievoudige doorgifte-transmissie van $\lambda = 1,000$ nm.

Een van de effecten die in de voorgaande hoofdstukken hebben bijgedragen aan slechte SAW-prestaties, wordt geïdentificeerd als de impedantie-mismatch tussen de IDT op het substraat en de RF-vermogensbron, die gematcht is met 50Ω . In **hoofdstuk 5** simuleren we numeriek het piëzo-elektrische substraat dat in voorgaande hoofdstukken werd gebruikt en passen we het toe op een IDT-equivalent circuitmodel voor het afstemmen van de elektrische impedantie. Het is gebleken dat de IDTs die worden gebruikt op het nano-imprintmasker in hoge mate elektrisch en akoestisch reflecterend zijn vanwege hun aanzienlijke lengte en het overeenkomstige hoge aantal vingerparen. De IDT-modelresultaten worden vergeleken met experimentele VNA-metingen in de hoofdstukken 3 en 4 en het model blijkt onvolledig te zijn aangezien het geen rekening houdt met de vele reflecties en resonanties die optreden in de gefabriceerde devices. Desalniettemin zijn de simulatie en het model een handig hulpmiddel voor het identificeren van mogelijke valse IDT-reacties en als een eerste benadering om impedantie-mismatch te minimaliseren.

De materiële oorsprong van voortplantingsverlies kan worden verminderd door het gebruik van materialen die tijdens de fabricage minder gevoelig zijn voor degradatie. Aluminiumnitride (AlN) is een hard piëzo-elektrisch materiaal met een hoge geluidssnelheid ($\approx 10,000 \text{ m s}^{-1}$), dat aantrekkelijk is voor toegang tot hogere frequenties zonder dat er kleine golflengten nodig zijn. In **hoofdstuk 6** wordt een nieuwe piëzo-elektrische dunne film, Sc-gedoteerd AlN, gedeponeerd op SiO_2/Si en geanalyseerd door middel van SAWs, welke zijn gegenereerd met NIL-gedefinieerde vertragslijnen. De generatie en voortplantingseigenschappen van SAWs opgewekt met behulp van deze dunne films worden geanalyseerd via een VNA en vergeleken met de piëzo-elektrische materialen beschreven in de voorgaande hoofdstukken. De SAW-transmissies blijken krachtiger en robuuster te zijn dan op ZnO lagensysteem, maar de aanwezigheid van ongewenste schuif- en bulkmodi kan een belemmering vormen voor een succesvolle toepassing in akoesto-elektronische apparaten.

Tot slot geeft **hoofdstuk 7** een perspectief op een nieuwe generatie silicium ACT-devices die de kennis en ervaring uit de voorgaande hoofdstukken van dit proefschrift gebruiken in hun ontwerp. Er wordt een nieuwe combinatie van dunne-filmmateriaal en fabricageproces voorgesteld om schade aan de piëzo-elektrische dunne-films, die in potentiële nieuwe devices worden gebruikt, te minimaliseren. Numerieke simulatie en het equivalente circuitmodel uit hoofdstuk 5 worden gebruikt om de ideale IDT-lengte te bepalen voor de voorgestelde nieuwe materiaalstructuur. Bovendien worden alternatieve IDT-ontwerpen geïntroduceerd voor verbeterde generatie en voortplanting van hoogfrequente SAWs met behulp van IDTs met grotere golflengtes.

PUBLICATIONS

R. Ukropec, B. Vratzov, P.V. Santos, W.G. van der Wiel, "High-frequency silicon opto-acousto-electronic devices", (manuscript in preparation).

R. Ukropec, B. Vratzov, W.G. van der Wiel, "High-frequency acoustic propagation loss on $\text{SiO}_2/\text{LiNbO}_3$ ", (manuscript in preparation).

R. Ukropec, D. Kooij, W.G. van der Wiel, "Impedance matching silicon SAW devices", (manuscript in preparation).

R. Ukropec, M.S. Lozano, G.F. Iriarte, W.G. van der Wiel, "Thin film ScAlN for ultra-high frequency silicon acoustics", (manuscript in preparation).

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