

École polytechnique de Louvain

Silicon-based Surface Acoustic Wave resonators for more sustainable RF integrated filters

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Chapter 1

Introduction

Electronic devices are taking more and more place in our lives and are becoming increasingly complex. The communication system, which is a key part of these devices, is becoming more efficient and smaller, and new technologies such as 5G are putting even more pressure on these devices. Specific technologies and materials are needed to meet the requirements for these huge performances. However, this comes at a cost, which is economic but also environmental and social, and cannot be neglected anymore.

This thesis is focused on piezoelectric resonators, which are the base elements used in filters for radio frequency communication. More specifically, surface acoustic wave (SAW) resonators are studied. These resonators are made of piezoelectric materials, materials which, thanks to their particular structure, have specific electromechanical properties which make them particularly suitable for this application. The focus will be set on three different technologies. Two of them are using the same piezoelectric material, lithium tantalate. The first technology uses a substrate made only of lithium tantalate, while the second technology, called piezo-on-insulator (POI), uses a multilayer substrate made of a thin layer of lithium tantalate on a silicon substrate, with both layers separated by an oxide layer. The alternative to lithium tantalate which will be studied is aluminium nitride.

Based on an analysis of both the performances and the sustainability of these three technologies, the aim of this thesis is to determine which is the most suitable for the SAW resonators of tomorrow.

This analysis will start by a context which outlines the motivation of this thesis. Then, a theoretical overview will be done to properly explain the state of the art and present the important concepts which must be known to understand the rest of the analysis. A chapter is dedicated to the method, which shows how the results are obtained, and defines the tools which are used. The results will then be shown, with some explanations and observations, both for measurements and simulations. The following chapter is solely dedicated to the sustainability aspect, using different indicators to compare as objectively as possible the impact of the different technologies. This chapter will be completed by some interpretations. Then, a discussion will be done to assess the results from the analyses, put together to try and come to a conclusion. The conclusion aims to answer the objective of this thesis.

Chapter 2

Context

Mobile telecommunications are an important part of our lives today. And the progress in this field does not seem to stop soon. With new technologies such as 5G appearing and the fact that the usable range of frequency becomes overcrowded, the requirements for filters contained in those devices are becoming increasingly difficult to meet. Indeed, because of the excessive use of telecommunication, some bands of frequency allocated to RF communication are extended. But these bands cannot overflow on the others. The bandwidth of filters must thus be wider and skirts must be steeper [1]. Adding to these high performances, filters must be stable over a range of temperature, and be extremely small. All materials are not suitable to build these filters. Fortunately, some materials are capable of reaching these requirements and new technologies are created for this purpose.

Surface acoustic wave (SAW) filters seem to offer a good solution to meet the requirements. The main objective of this work is to assess different substrate technologies for SAW resonators, which compose SAW filters. One of those technologies is a new technology created by Soitec, the so-called piezo-on-insulator (POI) substrate which is very promising. It uses a piezoelectric material, lithium tantalate, which is used since a long time in SAW devices [2]. Comparing these two technologies is an essential part of this work. Another technology for SAW filters is investigated: aluminium nitride (AlN). The properties and performances of these technologies will be evaluated and discussed.

Another motivation for this work is the fact that we are living nowadays in an ecological and social crisis. Indeed, lithium tantalate, which is a common substrate for SAW devices as mentioned, comes from materials which are becoming increasingly known as problematic. One of which is coltan, whose infamous mining is associated to dramatical geopolitical conflicts in Democratic Republic of the Congo (DRC). The other, lithium, is rapidly becoming a critical material for the world economy, due to the rise of electric vehicles and the requirements of their batteries. This boom comes with current and anticipated environmental and social concerns. Hence, POI and AlN are considered as potential alternatives to lithium tantalate. They could indeed be more sustainable, while maintaining the expected level of performance. The aim of this thesis is to assess this claim by investigating both the performances and the sustainability of these technologies.

Chapter 3

State of the art

This section aims to cover some of the theoretical background leading to the realization of this work. Starting from the front end module, filters will also be briefly discussed before moving on to resonators, which are the focus of this work. Piezoelectricity and its properties will also be discussed, with a particular attention to lithium tantalate, which is a material of significant importance in the context of this thesis.

3.1 Front end module

The front end module (FEM) is present in all connected devices such as smartphones, laptops, etc. The front end module contains the RF (radiofrequency) front end. The RF front end is the circuitry responsible for converting radio signals from antennas (at high frequency) to data usable by the device (near-zero frequency). This circuitry is rather complex, a schematic of the RF front-end is shown in figure 3.1. The module is composed of :

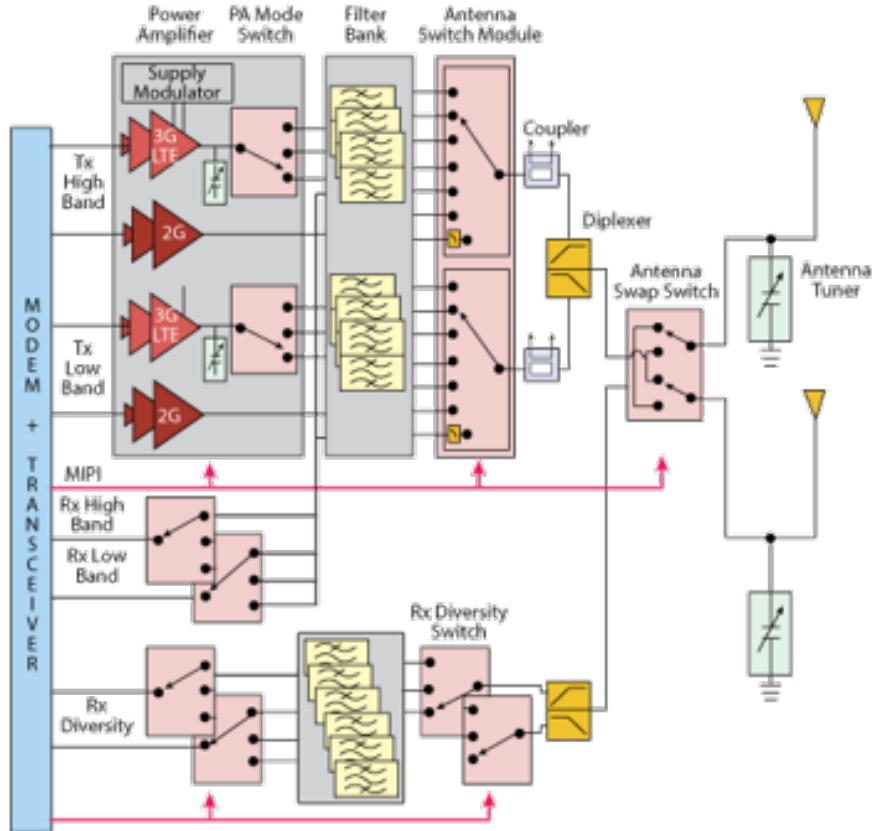


Figure 3.1: Schematic of the circuitry of a typical front end module [3]

- **Antennas** to transmit or receive information.
- **Switches** to provide the correct path to the signal.
- **RF Filters** (bandpass filters) which receive the signal from the antennas and remove all the unwanted parts of it such as image frequency and other out-of-band signals.
- **Amplifiers** which aim to amplify weak signals without creating additional noise.
- A **local oscillator** to generate a stable radio frequency.
- A **mixer** which produces a signal at a certain frequency by mixing the wave with the signal from the oscillator.

Figure 3.2 is a schematic of the operation of the front end module and RF front end module (red).

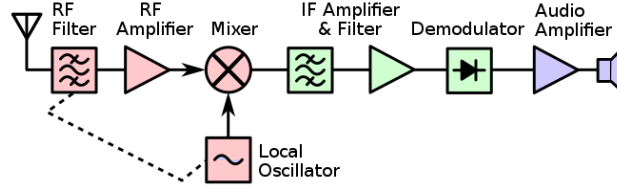
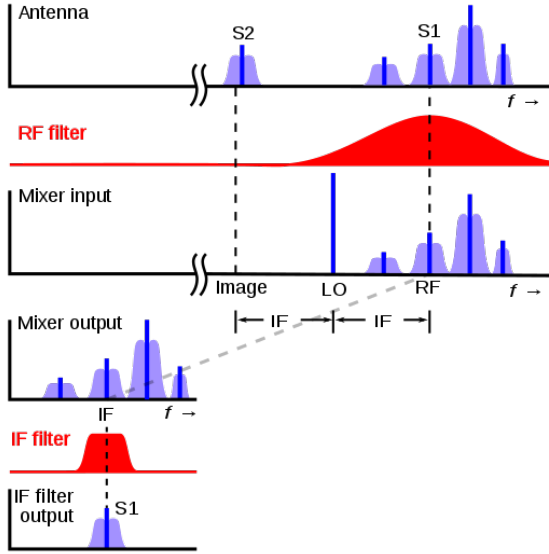
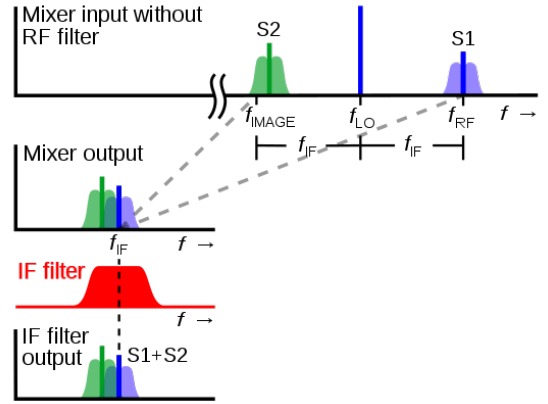


Figure 3.2: Working principle of the front end module with RF front end in red.



(a) Graph of the signal at different stages of the front end module. The x-axis is the frequency while the y-axis is the voltage of the signal.



(b) Problem of the image response. x-axis is the frequency while y-axis is the voltage of the signal [4].

Figure 3.3: Schematics explaining the working principle of FEMs [5]

The signal which comes from the antennas to the RF filter is rough. There can be unwanted or parasitic signals at any frequency. The goal of the RF filter is mainly to remove the image signal (S_2 on the graph in figure 3.3a). If this signal is not removed, it will be added to signal S_1 at the output of the mixer. This phenomenon is shown at figure 3.3b.

If we mix two signals S_1 and S_2 which have a frequency f_1 and f_2 respectively, the signal at the output of the mixer will have 2 parts: one at frequency $f_1 + f_2$ and the other at $|f_1 - f_2|$. Figure 3.3b can now be explained. Knowing that we want to catch the signal at frequency f_{RF} , the frequency of the local oscillator (f_{LO}) and the frequency of the intermediate frequency (IF) filter (f_{IF}) will be chosen such that $f_{IF} = f_{RF} - f_{LO}$ as the signal from the antennas will be mixed with the signal from the local oscillator. Unfortunately another signal will be present at frequency f_{IF} if nothing is done previously: the signal at frequency $f_{IMAGE} = f_{LO} - f_{IF}$. Indeed the mixing of this signal

with the signal from the local oscillator will give a signal centered at f_{IF} too and will thus be in the window of the next bandpass filter. This is why the RF filter is so important: to remove the image frequency. It is also useful to prevent strong out-of-band signals from saturating the input stages.

The multiplication of technologies such as 3G/4G/WIFI/GPS makes the front end module bigger and bigger and increasingly complex. This is exacerbated by 5G. The number of antennas, switches, filters, etc. is skyrocketing, and new challenges beckon for front end modules. In the context of this thesis, we are particularly interested in RF filters which are described in the next section.

3.2 Filters

As seen previously RF filters are a key part of the front end module. RF filters are bandpass filters which work at high frequency, typically in the GHz range.

In recent years, telecommunications have become increasingly fast and important. The creation of new technologies such as 5G requires new frequency bands and the existing frequency bands for mobile communication are extended or even newly defined with additional frequency ranges. The frequency spectrum which can be allocated for mobile communication becomes overcrowded. There are thus also more requirements for RF filters. They need a larger bandwidth (BW) and steeper skirts. An example is a current Band 25-long-term evolution (LTE) duplexer¹ [1] : Band 25 [transmitter (Tx): 1,850–1,915 MHz; receiver (Rx): 1,930–1,995 MHz] is an extension of Band 2 (Tx: 1,850–1,910 MHz; Rx: 1,930–1,990 MHz) by 5 MHz in each band. We need nearly 10 MHz more BW in the Tx as well as in the Rx band due to the larger nominal BW and the new channel requirements for LTE.

Other requirements for RF filters are: low insertion loss (IL, which is the ratio between the power of the signal without and with the filter in the frequencies of interest), high out-of-band suppression/attenuation both close to the passband and far from it (see figure 3.4), power durability, electrostatic discharge stability, and good nonlinear behavior. Furthermore the size of these filters needs to be as small as possible. As an example, the typical size of a Band-25 duplexer is 2-3 mm³.

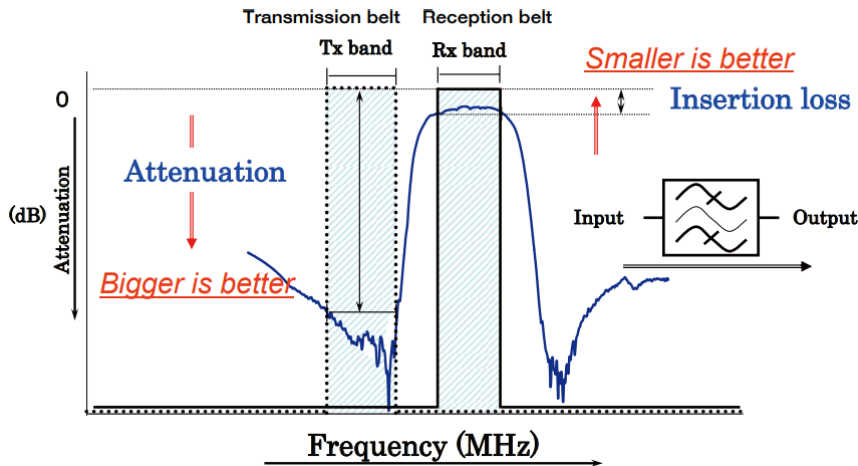


Figure 3.4: Illustration of the requirements of a RF filter [6]

The only type of technologies able to meet these requirements while displaying a small size are bulk acoustic wave (BAW) and surface acoustic wave (SAW) devices.

Both technologies are using piezoelectric materials and resonators which will be described in the following sections.

Currently, the range of frequency which is used for mobile communications is from the left edge of Band-12 Tx at 699MHz and right edge of Band-43 at nearly 4GHz. It is thus necessary to choose the adequate technology for each band. This choice is summarised at figure 3.5.

SAW filters are cheaper and easier to manufacture than BAW filters. But BAW filters exhibit

¹A multiplexer is built by several filters connected to one node, typically the antenna node. When two filters are

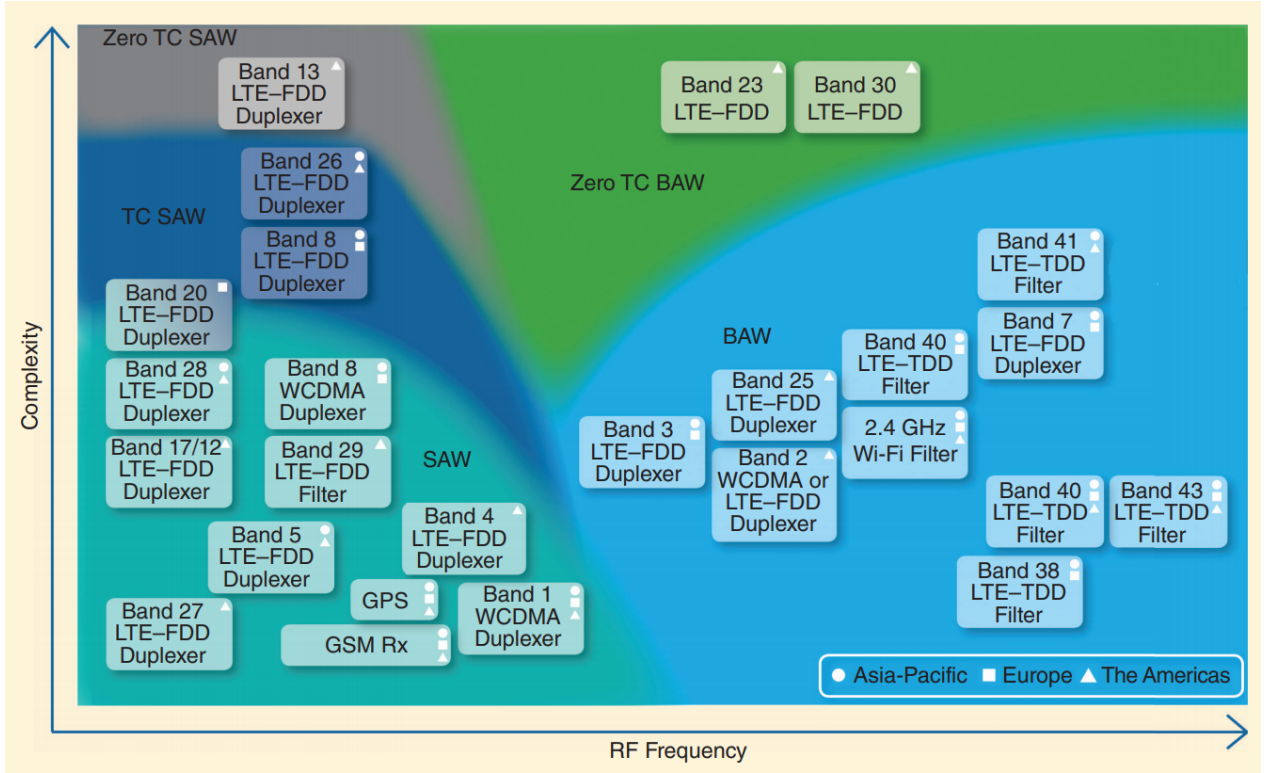


Figure 3.5: Matching filter technologies to mobile applications. FDD: frequency-division duplex; GPS: global positioning system; GSM: Global System for Mobile Communications; TDD: time-division duplex. [1]

higher quality factors which lead to lower insertion loss and higher steepness of skirts. Furthermore they have a lower (in magnitude) temperature coefficient of frequency (TCF, see section 3.4.4.4). SAW technology is thus used for low-band (< 1 GHz) with medium requirements for steepness of skirts and medium requirements for temperature shift. BAW technology is used from midband frequency (> 1.5 GHz).

Another technology was introduced: temperature compensated (TC) SAW. Indeed the TCF of lithium tantalate (LiTaO_3) is quite high when it is used as a substrate (-40 ppm/K). The idea is then to combine lithium tantalate with other materials which exhibit a positive TCF in order to reduce the magnitude of the TCF of the whole device. Typically silicon dioxide (SiO_2) can be used. This technology is suitable for bands more sensitive to temperature. But some bands require at least one skirt which does not move over temperature. It is possible with the same principle by adjusting the thickness of the SiO_2 layer.

The key element of the filters for each of these technologies is the resonator. Either bulk acoustic wave (BAW) resonators or surface acoustic wave (SAW) resonators. Resonators (especially SAW resonators which are the main topic of this thesis) will be more precisely described in the next section. The role of these resonators within filters is outlined here.

The symbol of a resonator (either BAW or SAW) is illustrated in figure 3.6a while the theoretical curve of its admittance is available in figure 3.6b. A resonator is characterized by: a resonance frequency f_r with a high admittance, and an antiresonance frequency f_a with a low admittance; as shown on the theoretical curve of the admittance.

Based on these resonators, filters can be implemented through basic architectures. There are often between 5 and 20 resonators (of the same type: BAW, SAW, TC SAW,...) per filter. The two main topologies will be briefly described here.

The first one is the ladder-type filter, consisting in an assembly of resonators in series and in parallel as shown in figure 3.7a. The working principle of the filter is shown in figure 3.7c. All resonators in series have the same resonance frequency f_r^S and antiresonance frequency f_a^S . All resonators in parallel have the same resonance frequency f_r^P and antiresonance frequency f_a^P . The

connected, it is called a duplexer, a quadplexer is formed with four filters, etc.

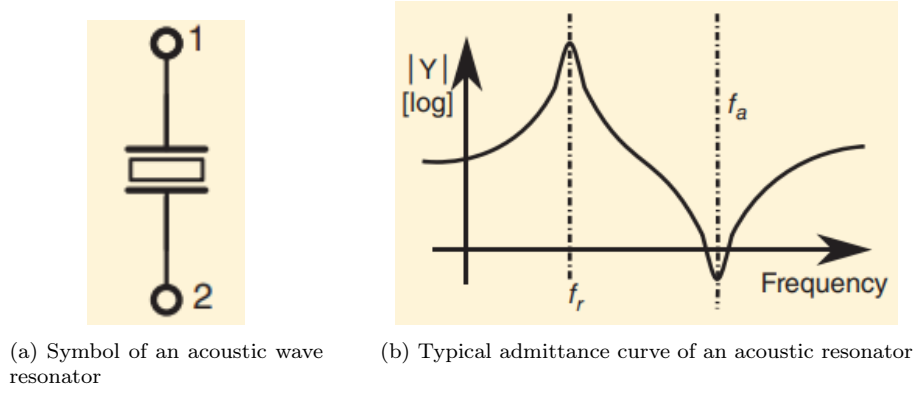


Figure 3.6: Basic figures of acoustic resonators [1]

best compromise between BW and good return loss (RL) within the band that also correlates with a flat passband is for the antiresonance frequency f_a^P of $P01$ and $P02$ to be somewhat lower than f_r^S [1]. This topology can be realized with both SAW and BAW resonators. In the circuit of figure 3.7a, only two series resonators and two parallel resonators are used. This example is called two-stage ladder filter. In order to have steep edges of the filters, it is often necessary to have more than three stages. Five stages is usually too big for the die size. Thus three and a half to four ladder stages are generally found in acoustic wave filters.

The second topology is the coupled resonator filter (CRF) and is shown at figure 3.7b. CRF is only used for SAW. It operates from single-ended to balanced mode. The design shown at figure 3.7b, one track with 5 IDTs CRF and a two-stage ladder filter at the input, is common because it leads to the best rejection and best compromise between insertion loss (IL) and stopband (SB) suppression.

The benefits of the CRF over ladder type filters are: smaller die size, and a higher SB suppression for the IL. Nevertheless, the power durability of the ladder type filter is greater.

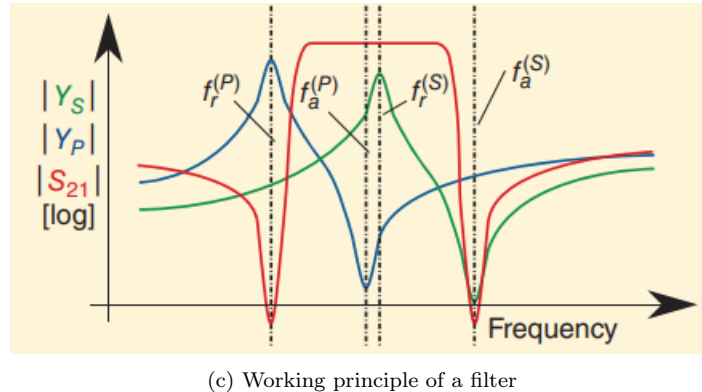
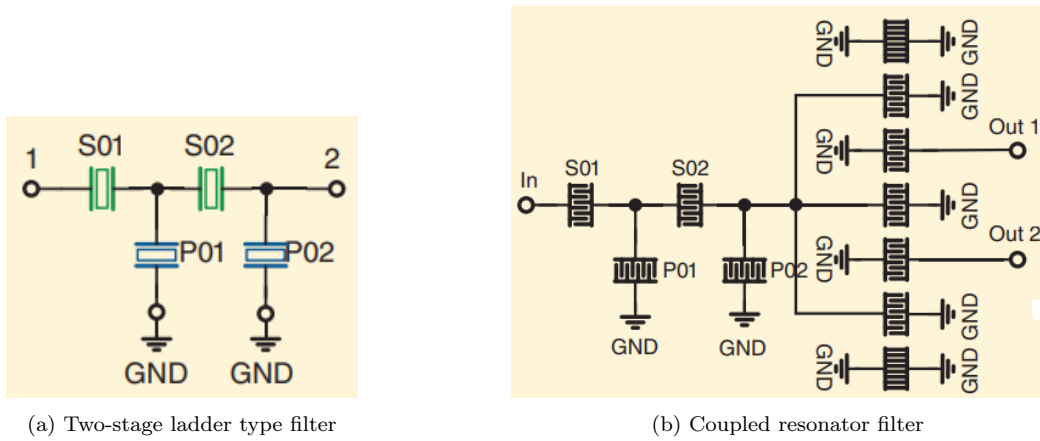


Figure 3.7: Filter topologies and working principle [1]

3.3 Piezoelectric materials

Piezoelectric resonators are the only technology available which meets the requirements of the front end module and RF filters (see section 3.2). In order to properly understand the operation of these resonators, a clear comprehension of the piezoelectric materials is necessary.

Piezoelectric materials are important in the context of resonators as they allow efficient designs with very high quality factor and sharp resonance for a small surface. This constitutes the main use of piezoelectric materials in RF applications. Piezoelectric materials are defined by several physical properties including: piezoelectric constants, stiffness, and dielectric constants (or relative permittivity).

3.3.1 Principle of piezoelectric materials : constitutive equations

The key principle of piezoelectricity is the coupling between electric fields and displacement on one hand and elastic stresses and strains on the other hand. It only occurs in anisotropic materials, and in most cases its effect is negligible. However, in the context of resonators, we are studying materials used specifically to take advantage of their piezoelectric effect.

At each point of a homogeneous piezoelectric insulator, the stress tensor T depends not only on the stress tensor S but also on the electric field E .

$$T_{ij} = \sum_k \sum_l c_{ijkl}^E S_{kl} - \sum_k e_{kij} E_k \quad (3.1)$$

In this equation, c_{ijkl}^E is the stiffness tensor for a constant electric field, e_{kij} is the piezoelectric tensor (a tensor of piezoelectric constants) relating elastic fields to electric fields, and the quantities are assumed to be small enough for this relationship to be considered linear.

Similarly, the electric displacement D can be determined from the electric field E and the strain S .

$$D_i = \sum_j \varepsilon_{ij}^S E_j + \sum_j \sum_k e_{ijk} S_{jk} \quad (3.2)$$

where ε_{ij}^S is the permittivity tensor for constant strain and e_{ijk} is the piezoelectric tensor.

The electric displacement field D can also be expressed depending on the stress T rather than the strain S .

$$D_i = \sum_j \varepsilon_{ij}^T E_j + \sum_j \sum_k d_{ijk} T_{jk} \quad (3.3)$$

In that case, ε_{ij}^T is the permittivity tensor for constant stress. The tensor d_{ijk} is more complicated to define. It is possible to obtain an expression of T in terms of S_{kl} and D from equations (3.1) and (3.2). The coefficients of S_{kl} then give a stiffness tensor for constant electric displacement [7].

3.3.2 Loss mechanisms in piezoelectric materials

Performances of piezoelectric devices depend on the two-way coupling between stress and electric field, in other words on the conversion from electrical to mechanical energy and vice-versa. The efficiency of this conversion therefore needs to be quantified. Figures of merit such as the electromechanical coupling factor and the quality factor serve that purpose, and will be described later on. In order to understand the physical origins of this conversion efficiency, it is necessary to introduce loss mechanisms occurring inside piezoelectric materials. Three sources of loss can be identified : electrical losses, mechanical or elastic losses, and coupling or piezoelectric (thus electromechanical) losses. Losses can also be further classified into intrinsic (fundamentally related to material properties) and extrinsic (dependent on the design and implementation of the piezoelectric device) losses.

3.3.2.1 Electrical losses

When discussing electrical losses, dielectric loss is the main mechanism at work in piezoelectric materials, which are also dielectric. Dielectric losses are associated with heat generation in the

static capacitances of the device. Piezoelectric materials are polarized by the electric field due to the coupling with the stress field. Energy is stored in the form of charges on metallic electrodes. The polarization process involves a movement of centers of charges in the material. During this movement, dielectric relaxation occurs : some of the applied energy is directly transformed in heat and is therefore lost [8].

Dielectric losses are described by a material constant called loss tangent :

$$\text{tg } \delta = \frac{\epsilon''}{\epsilon'}$$

where

- δ is the loss factor (lower loss tangent means lower dielectric loss, which is desirable)
- ϵ' and ϵ'' are real and imaginary parts of the complex permittivity : $\epsilon = \epsilon' - j\epsilon''$.

Dielectric losses are intrinsic, they depend on the piezoelectric material itself.

Ohmic losses are other electrical losses occurring in piezoelectric resonators. The thin films of metal used as electrodes constitute considerable resistive loads where electrical energy is lost as heat. These losses are extrinsic, they depend on the shape of the material. Thicker layers (which have lower resistivity) can be used to alleviate these losses.

3.3.2.2 Mechanical losses

Mechanical, acoustic or elastic losses include mechanisms of conversion of mechanical energy into heat, or leakage of mechanical energy from the device.

Damping is the main source of mechanical losses. Damping has a strong effect on structures subject to harmonic excitation at a frequency close to their natural frequency. At resonance, the vibration amplitude tends to infinity in theory, but in practice it has a finite value because of damping. The mechanical Q factor (or quality factor) is a measure of damping. It is the amplification at the resonance, and is thus particularly important for applications such as resonators, which aim to get the biggest amplification possible. The Q factor can be defined as

$$Q = \frac{1}{2\zeta\sqrt{1-\zeta^2}} \approx \frac{1}{2\zeta}$$

ζ is the damping ratio, which can be derived from the equation of motion for a system with one degree of freedom with viscous damping and no external load ($\sum F = 0$) (3.4).

$$m\ddot{u} + c\dot{u} + ku = 0 \quad (3.4)$$

In this equation, m is the mass, c the viscous damping coefficient, k the stiffness constant, u is the displacement, $\dot{u}$ is the velocity, and $\ddot{u}$ is the acceleration. The normalized version of equation (3.4) is obtained by dividing it by the mass m :

$$\ddot{u} + 2\zeta\omega_0\dot{u} + \omega_0^2u = 0$$

where ω_0 is the undamped natural angular frequency. The damping ratio ζ is limited to the range $0 \leq \zeta < 1$ in order for the motion to be periodic. The amplitude of vibration of the system will decay with a factor $e^{-\zeta\omega_0 t}$.

Damping can also be described using complex material properties, in similar fashion as the dielectric losses. The stress-strain relation for uniaxial linear elasticity can be written as :

$$\sigma = E\varepsilon = (E' + iE'')\varepsilon$$

with stress σ , strain ε , and Young's modulus E which is separated into real and imaginary parts called storage modulus E' and loss modulus E'' , respectively. The loss modulus is often described by a loss factor η :

$$E = E'(1 + i\eta)$$

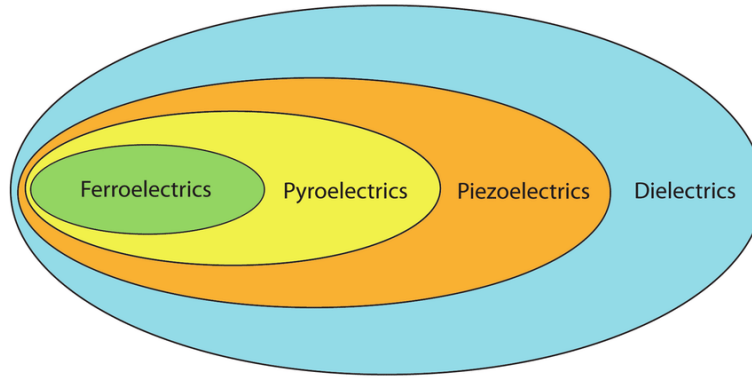


Figure 3.8: Relationship between dielectric, piezoelectric, pyroelectric and ferroelectric materials [12]

Loss factor damping can be measured, much like dielectric losses, as a loss tangent :

$$\tan \delta = \frac{E''}{E'} = \eta$$

where loss angle δ is the phase shift between stress and strain, which forms a hysteresis loop over a complete period [9].

There are other, less important types of mechanical losses such as phonon-phonon interaction, which can cause losses of vibrational energy.

3.3.2.3 Electromechanical losses

Electromechanical, piezoelectric or coupling losses are associated with the non-ideal mutual conversion of mechanical and electrical energy. This category of losses is the last to have been recognized as an independent source of losses and the origins of these losses are not fully understood. Researchers have suggested to extend the complex representation of material properties to the piezoelectric constants. Piezoelectric losses are thought to be a result of damped motion of domain walls in ferroelectrics [8].

3.3.3 Pyroelectricity

Pyroelectricity is the ability of certain materials to generate an electric polarization when they are heated or cooled [10]. Pyroelectricity occurs in all materials that belong to a polar crystal symmetry class, while piezoelectricity occurs in all noncentrosymmetric materials [11]. As not all noncentrosymmetric classes are polar, not all piezoelectric crystals are pyroelectric, however all pyroelectric crystals are piezoelectric. Furthermore, ferroelectrics form a subset of the set of pyroelectrics because they are polar materials in which the direction of the polar axis can be changed by the application of an electric field. The relationship between these type of materials is summarized in figure 3.8.

Pyroelectricity is not to be mistaken for thermoelectricity, which is the generation of a stable electrical potential in a fixed temperature profile. In pyroelectricity, a change in temperature attracts electrons from the ambient to the surface of the material due to changes of polarization in the material. Whereas in thermoelectricity, electrons or holes travel within the material, generating an electrical current [13].

3.4 Resonators

RF filters are made from a combination of acoustic resonators. All technologies of acoustic resonators take advantage of the piezoelectric effect of certain materials. The main figures of merit for piezoelectric resonators are the quality factor Q and the coupling factor (usually squared) k^2 . These values will be observed around the resonance frequency, which is also a parameter studied to

assess the performance of piezoelectric resonators. Maximum frequency of operation, ability to hold up high RF power, electromechanical factor and deposition process are all parameters that will be looked at by end-users [14]. There are two main kind of acoustic resonators: bulk acoustic wave (BAW) resonators, and surface acoustic wave (SAW) resonators. The working principle of these two technologies is described in this section with a focus on SAW resonator which is the topic of this thesis.

3.4.1 BAW resonators

The basic principle of a BAW resonator is to excite a film of piezoelectric material via two electrodes: one above and the other below the film (the piezoelectric material is sandwiched between the electrodes). The wave is thus propagating inside the piezoelectric film. The fundamental resonance occurs when the wavelength of the mechanical wave is twice the thickness of the film [15] as shown in equation (3.5) :

$$f_0 = \frac{v}{2d} \quad (3.5)$$

With f_0 the fundamental frequency, v the acoustic velocity, and d the thickness of the film.

Electrode thickness can also have an impact on the resonance frequency. Indeed, the mass of the electrode can generate a frequency shift.

Different topologies of BAW resonators exist. Some examples are shown in figure 3.9.

The structures shown in figures 3.9a and 3.9b are two examples of Film Bulk Acoustic Resonator

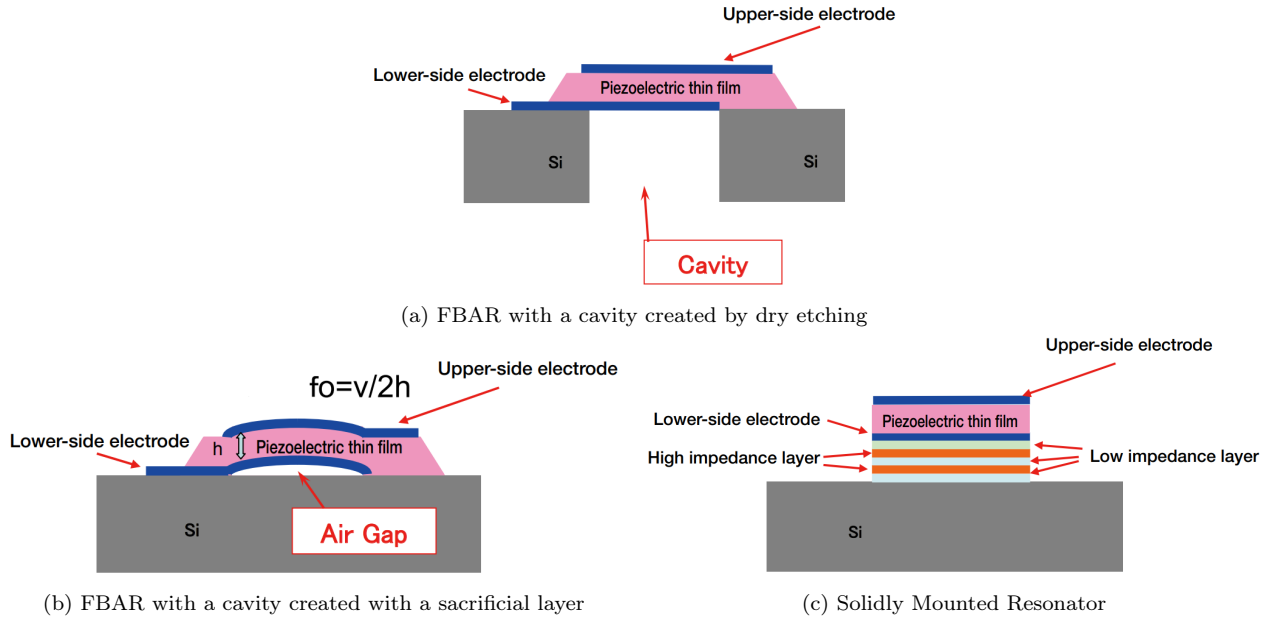


Figure 3.9: Different topologies of BAW resonators [6]

(FBAR). They are BAW resonators built on cavities. The cavity can be made by dry etching of silicon as in figure 3.9a or with a sacrificial layer which is removed as in figure 3.9b.

The structure shown at figure 3.9c is another kind of BAW resonator which is the Solidly Mounted Resonator (SMR). This structure works with a Bragg reflection layer. The goal of this layer is to reflect the bulk acoustic wave so that it does not leak in the substrate. The Bragg reflection layer is formed by an alternance of high and low impedance layers. Each layer is one quarter of wavelength thick.

BAW resonators will not be described further in this work as the focus is on SAW resonators.

3.4.2 SAW resonators

SAW resonators are using interdigital transducers (IDTs) placed on the top surface of a piezoelectric material in order to excite surface acoustic waves. The schematic of the basic structure of a SAW

resonator is shown in figure 3.10a. The basic component of SAW resonators is the IDT, made of interlocking comb-shaped electrodes (figure 3.10b). Besides, reflectors (sometimes called mirrors) are located at both ends of the resonator. Their purpose is to reflect the wave in order to avoid losses. Indeed, acoustic waves can be reflected by a solid surface. The wave reflected by one reflector finger interferes with the incident wave and with the waves reflected by the other reflector fingers. Only part of the wave is reflected by a reflector finger. Hence an array of fingers is used in order to achieve the reflection of almost the entirety of the wave, thus effectively limiting losses. The wave decays exponentially in the reflector array, so that a finite number of fingers is sufficient to reflect the majority of the wave. Both IDTs and reflectors are made of metal, such as aluminium.

The period of the IDT has a length λ , which corresponds to the wavelength of the acoustic wave (figure 3.10b); a common practice is to select $\lambda/4$ as the width of the fingers and the spacing between fingers. As reflected waves must interfere constructively, the period of a reflector must be a multiple of $\lambda/2$. Usually, the reflector period is simply $\lambda/2$ in order to minimize its size. Furthermore, the spacing between the IDT and the reflector also needs to be a multiple of $\lambda/2$ to ensure constructive interference, with $\lambda/2$ being the common option.

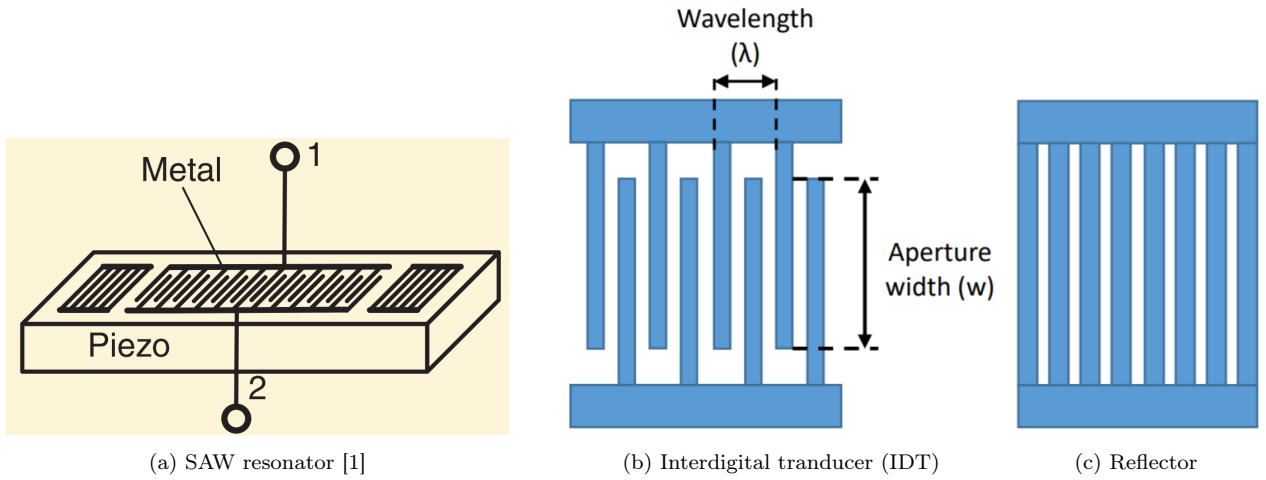


Figure 3.10: SAW resonator and its basic components

As in the case of BAW resonators, a fundamental resonance can be found. However, the resonance frequency of SAW resonators does not depend on the thickness of the piezoelectric material (as it does with BAW resonators) but rather on the period of the IDT, as is shown in equation (3.6).

$$f_0 = \lambda \times v \quad (3.6)$$

With f_0 the resonance frequency, λ the wavelength (determined by the period of the IDT) and v the acoustic velocity of the surface acoustic wave, which depends on both the material and the type of wave.

3.4.3 Surface acoustic waves in piezoelectric materials

A multitude of acoustic waves can be present in piezoelectric materials. Each application is designed to select or isolate the relevant type of wave. One important aspect of wave properties in piezoelectric materials is that they depend on the crystal orientation, which is outlined first in order to allow a proper comprehension of the different type of waves. Then, plane waves in anisotropic materials are also introduced as they are important to understand surface waves types. Finally, the relevant types of surface waves encountered in piezoelectric materials are briefly presented.

3.4.3.1 Crystal Orientation

As piezoelectric materials are anisotropic (piezoelectricity can only occur in crystals lacking a center of symmetry), their properties are affected by the crystal orientation, which therefore needs to be

taken into account carefully. This is especially true about lithium tantalate, which notoriously has a behaviour strongly depending on crystal orientation. As such, there exists some preferred orientations in research, and $42^\circ\text{Y-X LiTaO}_3$ is one of them. The specifications preceding the name of the material (in this case, " 42°Y-X ") give two important pieces of information. The first part, before the hyphen, specifies the outwardly directed normal to the surface (the surface of interest regarding wave propagation, that is, the wafer top surface) which is usually referred to as x_3 [7]. The second part, after the hyphen, specifies the propagation direction of the wave, usually referred to as x_1 . Axes x_1 and x_3 are illustrated in figure 3.12. They form what is called the sagittal plane.

In this case, " 42°Y " means that the cutting plane of the wafer is normal to a new axis Y' which is the result of a 42° rotation with respect to axis Y , in the direction of Z , with X as the axis of rotation. As specified in the name, " X " is also the propagation direction of the wave. This is illustrated in figure 3.11a where it is also shown that axis Y' is the axis along which the crystal ingot has been grown. Figure 3.11b shows the resulting axes on a typical wafer of 42° Y-cut LiTaO_3 . Wafer manufacturers usually specify the orientation of the wave propagation direction with respect to the wafer flat, which serves as reference for fabrication processes.

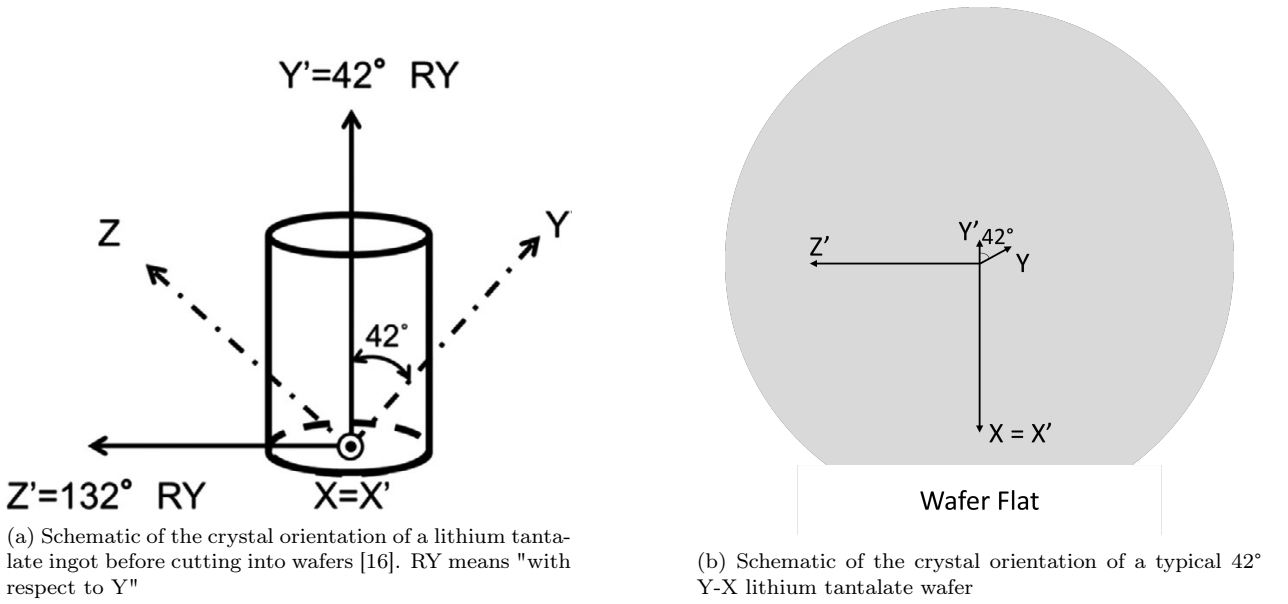


Figure 3.11: $42^\circ\text{Y-X LiTaO}_3$ cutting plane illustration

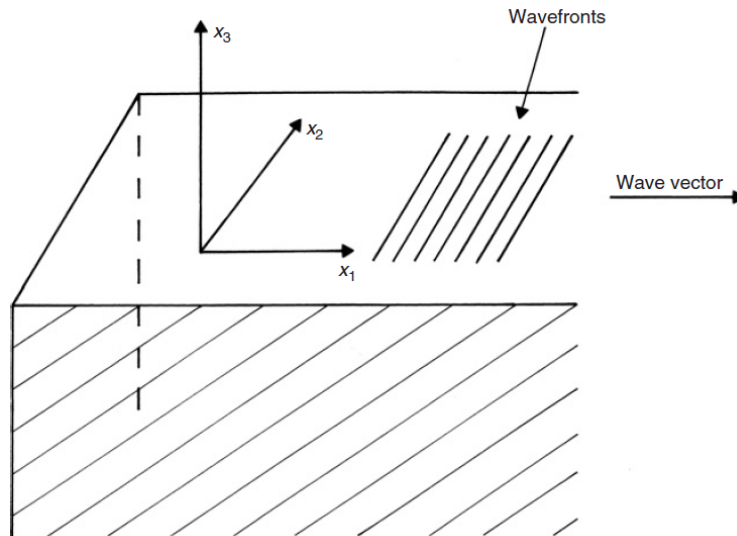


Figure 3.12: Representation of a half-space, with axes used to describe the propagation of acoustic waves [7]

3.4.3.2 Plane waves in anisotropic materials

All types of waves described in this section are solutions (also called modes) of the mechanical equation of motion valid for piezoelectric materials (which are anisotropic), the derivation and resolution of which will not be addressed here as it is beyond the scope of this work. The resolution of the equation of motion is especially complex for anisotropic materials, which is why isotropic counterparts are often used to facilitate its understanding. It should be noted that the equation of motion of piezoelectric materials depends on four quantities: the three components of displacement u_i and electric potential ϕ . From there, boundary conditions can be applied to define specific situations, with the solutions satisfying those conditions being existing wave modes.

The most basic situation is simply the one without boundary conditions, which is the infinite medium. In this case, one solution is electrostatic in nature and therefore non piezoelectric (piezoelectric tensor $e_{ijk} = 0$), which is of little interest for our work. The other three solutions are plane waves with distinct displacement. One is longitudinal and the other two are shear waves, with different velocities. Those two plane shear waves are named "slow" and "fast" and are used as reference for the phase velocity of surface waves described in this section. The displacement velocity depends on the propagation direction, because of anisotropy [7].

3.4.3.3 Types of surface acoustic waves in anisotropic materials

When talking about surface acoustic waves, we study waves that are propagating on the free surface of a semi-infinite body (also called half-space, illustrated in figure 3.12). Solutions to the equation of motion must therefore satisfy boundary conditions applied at the surface of the half-space, both in terms of force and electrical conductivity. The resulting modes are mostly confined near the surface, with displacement in the direction normal to the surface decaying exponentially. The main types of such waves are presented in this section.

Rayleigh waves Rayleigh waves are the most common type of surface acoustic waves and also the first to have been discovered. In fact, in many cases "SAW" refers to Rayleigh waves. Rayleigh waves display a combination of longitudinal and transverse (or shear) motion, with its displacement contained in or near the sagittal plane. Their velocity is slower than that of the slow plane shear wave [7]. An illustration of the propagation of a Rayleigh wave (in isotropic media) is provided in figure 3.13a. Rayleigh waves occur in both isotropic and anisotropic materials (such as piezoelectric materials), although there are some variations in behaviour due to piezoelectricity, which will not be covered in this work. Rayleigh waves are often exploited in SAW resonators and filters. Typical substrates using this type of wave are 128°Y-X lithium niobate and X-112°Y lithium tantalate.

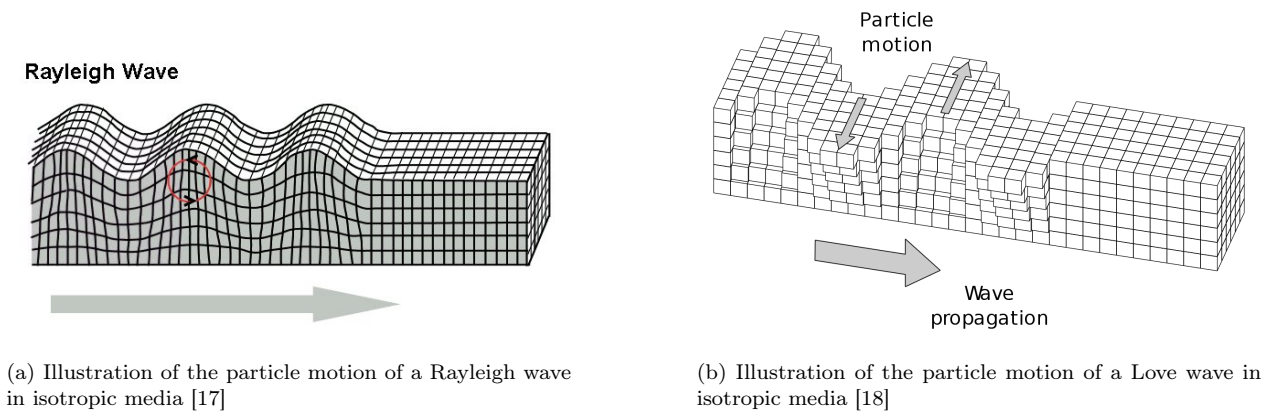
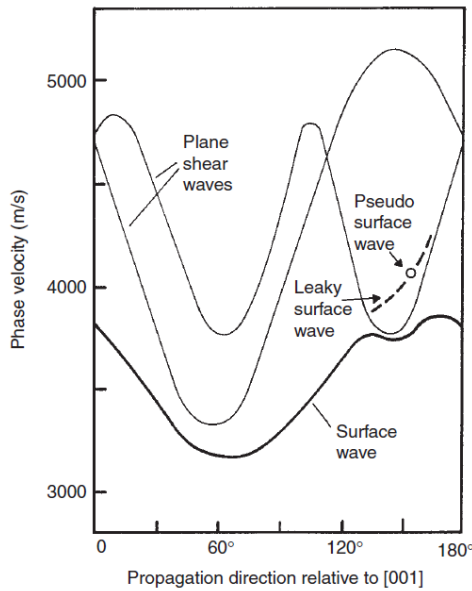


Figure 3.13: Particle motion of two common types of SAW in isotropic media

Bleustein-Gulyaev waves Bleustein-Gulyaev waves correspond to a solution occurring in a specific case: when the sagittal plane is normal to an even-order axis of the crystal. The resulting

wave has a displacement normal to the sagittal plane. The isotropic counterpart of Bleustein-Gulyaev waves is the shear horizontal plane wave, or the Love wave in a layered half-space. The particle motion of a Love wave is illustrated in figure 3.13b. It is in fact the piezoelectric effect that causes the wave to become bound to the surface in the case of a Bleustein-Gulyaev. Its velocity is close to that of the slow plane shear wave [7].

Leaky waves For propagation in a slightly different direction than in the Rayleigh case, a partial wave corresponding to the slow plane shear wave, which is usually a bulk wave needs to be included to satisfy boundary conditions. This means that energy is carried away from the surface and towards the bulk of the material, causing attenuation. When this attenuation is small enough that the wave behaves such as a surface wave, we talk about leaky waves (LSAW), as some energy is "leaked" or lost to the bulk. A particular case of leaky waves are pseudo-surface acoustic waves (PSAW) which have no attenuation as their displacement is perpendicular to the sagittal plane. The specificity of LSAW and PSAW is that they display a phase velocity higher than the slow plane shear wave, and thus higher than Rayleigh waves or Bleustein-Gulyaev waves, although lower than the fast plane shear wave [7]. Figure 3.14a shows the difference in phase velocity of the waves mentioned in this section, while figure 3.14b provides a summary table of those wave types.



(a) Phase velocity of different types of piezoelectric surface waves, depending on their propagation direction [7].

Table 2.1 Summary of wave types.

Isotropic half-space		Anisotropic half-space
Non-layered	Layered	
Rayleigh wave	Rayleigh wave (dispersive)	Rayleigh wave Pseudo-surface wave Leaky surface wave
SH plane wave	Love wave SH (dispersive)	Bleustein–Gulyaev wave

(b) Summary of the main types of surface acoustic waves [7]

Figure 3.14: Main types of surface acoustic waves and their phase velocity in anisotropic materials [7]

Leaky SAW possess several advantages for use in SAW devices such as resonators and filters :

- They have a high velocity, which is suitable for high-frequency applications.
- Their piezoelectric coupling is better than that of other surface waves. Their large electromechanical coupling coefficient allows a relatively wide passband which is required in recent mobile telecommunications technology [6].
- Their temperature stability is equal or better than that of other surface waves.

However, there is one key aspect of LSAW which cannot be overlooked: the low attenuation is only valid for specific orientations, which makes the performances of LSAW devices very sensitive to misorientation. This will be discussed later in this work. LSAW have been exploited with perovskites substrates such as 36° and 42°Y-X lithium tantalate or 64°Y-X lithium niobate. We are interested in this type of wave in this thesis, with 42°Y-X LiTaO₃ the main piezoelectric material used.

3.4.4 Figures of merit (FoM)

In order to have a clear comparison between several resonators it is important to define the figures of merit of a resonator. The main figures of merit are explained in this section.

3.4.4.1 Quality factor

The quality factor is a dimensionless parameter which reflects the losses of the system. The lower the losses, the higher the quality factor. There are several loss mechanisms, some losses are due to the piezoelectric material (described in section 3.3.2), but other losses can be possible such as ohmic losses for example.

A high Q-factor will induce a sharp peak at resonance and anti-resonance in the admittance plot (versus frequency) of the resonator. It will induce low IL and high steepness of skirts in the filter. The quality factor at resonance and anti-resonance is thus an important figure of merit for the resonators. There are several ways to compute the quality factor, which are described in section 4.

3.4.4.2 Effective electromechanical coupling factor (k_{eff}^2)

The effective electromechanical coupling factor k_{eff}^2 is a dimensionless parameter which quantifies the energy conversion of a piezoelectric resonator.

It is important to know that the effective coupling factor of a piezoelectric resonator (k_{eff}^2) is different than the coupling factor of a piezoelectric material (K^2). Indeed K^2 only depends on the piezoelectric material while k_{eff}^2 depends on the whole device, including the design of the resonator. We begin with the computation of the coupling factor K^2 . It is a unitless value used to quantify the efficiency of a piezoelectric material to convert electrical energy to mechanical energy. It can be translated mathematically as [8]:

$$K^2 = \frac{W_M}{W_M + W_E} \quad (3.7)$$

With W_M the mechanical work delivered by an actuator electrically loaded with potential energy $W_M + W_E$.

This ratio can be expressed as a function of material properties as in equation (3.8).

$$K^2 = \frac{e^2}{c^E \epsilon^T} \quad (3.8)$$

With e the piezoelectric constant, c^E the stiffness at zero electric field, ϵ^T the dielectric constant in the direction of the electric field at zero stress.

Each constant can be understood rather intuitively. The strong dependency (second-order) of the piezoelectric constant was expected because it is this coefficient that relates stress from mechanical domain to electric field in electrical domain. The effect of the stiffness can be seen as: the higher the stiffness constant, the smaller the mechanical displacement for a unit applied electric field (less displacement results in less mechanical work delivered to the load). This is why the stiffness constant is at the denominator. It is the same principle for the dielectric constant : the higher the dielectric constant, the larger the portion of total potential energy converted into electrical domain (not converted into mechanical energy). The dielectric constant is thus naturally at the denominator too.

This piezoelectric coupling factor K^2 is the maximum of the energy conversion efficiency in a resonator which uses a certain type of piezoelectric material. In other words, the effective coupling factor k_{eff}^2 which also depends on the design of the resonator will always be smaller than the coupling factor K^2 of the piezoelectric material which composes the resonator.

The computation of this effective coupling factor is shown in equation (3.9):

$$k_{eff}^2 = \frac{f_a^2 - f_r^2}{f_a^2} \quad (3.9)$$

With f_a and f_r the antiresonance frequency (frequency with the lowest admittance) and resonance frequency (frequency with the highest admittance) respectively.

3.4.4.3 Resonator FoM

Combining these two figures of merit (Q-factor and k_{eff}^2), a new figure of merit was created. The way to compute this figure of merit is shown at equation (3.10).

$$FoM = \frac{k_{eff}^2 Q}{1 - k_{eff}^2} \approx k_{eff}^2 Q \quad (3.10)$$

The approximation can only be done when the effective coupling factor is small (a few %), which is often the case.

A large effective coupling factor is due to an efficient mutual conversion of electrical to mechanical conversion. A large quality factor signifies low losses or in other words a weak coupling between the energy of the system and the undesired form of energy. A large FoM thus leads directly to a better signal-to-noise ratio which is the ultimate figure of merit for electrical systems [8].

3.4.4.4 Temperature coefficient of frequency (TCF)

Reliability of micro-electronic devices is one of the most important issues in mobile communication systems and is significantly influenced by the thermal behavior of the components [19]. Indeed, as explained in section 3.2, some bands need to be stable and skirts cannot move over temperature.

In order to quantify the shift of frequency with respect to the temperature, the figure of merit which is used is the temperature coefficient of frequency (TCF) which is expressed in [ppm/K]. The computation of the TCF is shown in equation (3.11)

$$TCF = \frac{1}{f} \frac{df}{dT} [ppm/K] \quad (3.11)$$

Typically the TCF of lithium tantalate is more or less -40 ppm/K while the TCF for BAW filters is between -27 and -18 ppm/K [1].

3.5 Technologies of interest

This section presents the materials used throughout this work. These materials compose the wafers used to fabricate the resonators, and thus also acts as substrates for the resonators. These materials will frequently be called "substrate technologies", "wafer technologies" or simply "technologies". This denomination helps distinguish those compound, end product technologies from the raw materials used to produce them. Three wafer technologies are used in our work : bulk lithium tantalate (LT), pizeo-on-insulator (POI) and bulk aluminium nitride (AlN).

3.5.1 Lithium tantalate (LT)

Lithium tantalate (LiTaO_3) is a perovskite ceramic of crystal structure 3m. It is well-known as a ferroelectric (and therefore pyroelectric, piezoelectric and dielectric) since 1949 [20]. It has been extensively studied because of its excellent piezoelectric, pyroelectric and optical properties. Its high quality factor and low acoustic losses make it an excellent material for high-frequency transducers and SAW devices. It also has a high Curie temperature, and shares these qualities with parent compound lithium niobate (LiNbO_3) [2]. While most things about lithium tantalate hold true for lithium niobate, the latter will not be discussed in this work.

The LT used in this work is more specifically 42°Y-X LT (the orientation notation is explained in section 3.4.3.1), which is particularly advantageous for SAW applications. Indeed, leaky SAW have a high velocity on such substrates, up to $4000\text{-}4200$ m/s [21] [22].

LT is not found in nature, and is therefore always synthetic. It is produced by the Czochralski method [20]. This notorious method permits the growth of a single crystal ingot, also called boule,

which can then be sliced into wafers. The method requires a crystal precisely oriented seed crystal which is mounted on a rod, and is dipped into a crucible containing molten material. The rod is then pulled out and a cylindrical single crystal boule is formed [23]. This method is also used for the production of other types of wafers, with the most common being silicon wafers. Figure 3.15 depicts the steps of the Czochralski process in the case of silicon. The same process is also valid for LT.

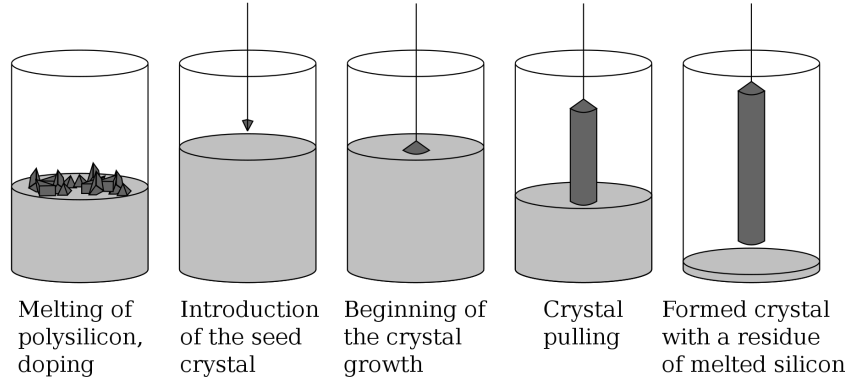


Figure 3.15: Czochralski process : detail of the steps for the production of a silicon boule [23].

3.5.2 Piezo-on-insulator (POI)

The piezo-on-insulator (POI) technology was created by Soitec some years ago. The goal is to fabricate resonators for filters which meet the requirements necessary for 5G front-end modules [24]. The design of the POI substrate is shown at figure 3.16.

This technology is supposed to bring a lot of benefits. According to Soitec, the buried oxide selects and guides only high velocity waves, allowing for low loss and very high signal selectivity. It also keeps the piezo material constrained against temperature variations, ensuring outstanding frequency stability when temperature changes [25].

The principle of POI is to improve the Leaky-SAW resonator by using guided waves that do not suffer from any radiation leakage. It enables guided modes within the top piezoelectric layer, yielding high quality factors since the acoustic energy is confined [26]. Furthermore, by combining LT with other materials as silicon oxide and silicon, the TCF can be decreased or even reduce to zero. Indeed the LT has a quite high TCE, responsible for a high TCF too (≈ -40 ppm/K). By combining LT with SiO_2 ($\text{TCE} < 1.5$ ppm/K) and Si ($\text{TCE} \approx 2.5$ ppm/K), TCF of the whole device is reduced too, below 10 ppm/K following a study from Soitec [27]. By controlling the thicknesses of different layers, TCF can be equalized to zero.

Here are the interests of waveguide structures [28] :

- suppression of radiation losses
- using shear waves expected to reduce intrinsic losses
- improvement of the coupling
- reduction of thermal expansion and TCF
- possible mode acceleration (to increase frequency)
- substrate linearity, resistivity, thermal conductivity and compatibility with CMOS electronics

Such a result is obtained thanks to a process invented by Soitec. The principle of this process is to implant ions in the wafer. Then a silicon wafer (grown with Czochralski process) is bonded

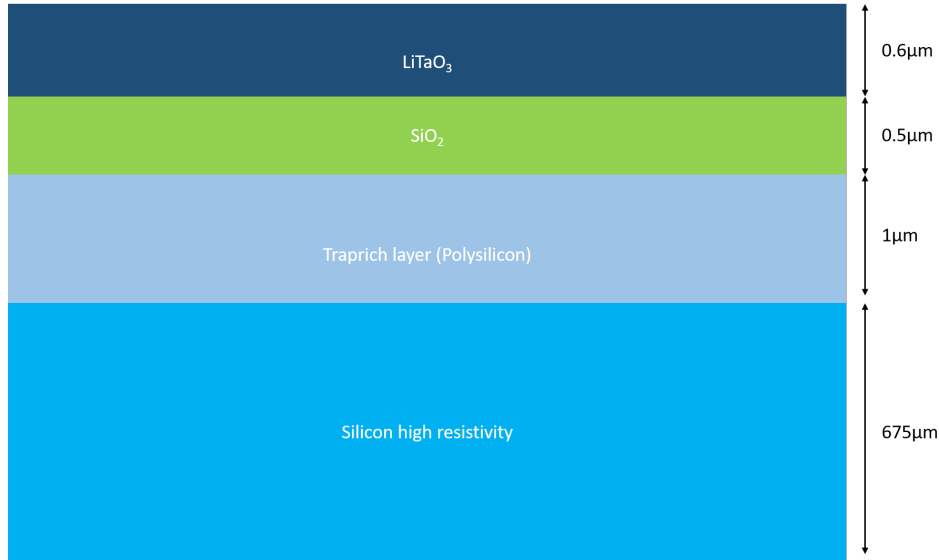


Figure 3.16: Side view of the POI wafer

to the LT wafer. The piezoelectric (LT) wafer will then be cleaved thanks to the effect of the ions. The part of wafer which is not used can become the base of the next POI wafer. A schematic which shows the principle of the Smart-cut is presented at figure 3.17.

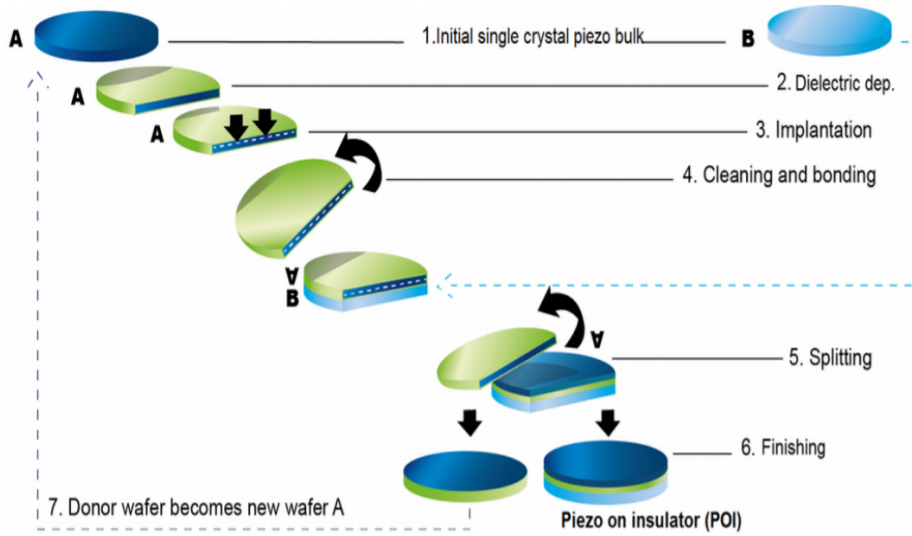


Figure 3.17: *Smart cut*TM principle and processing flow chart for POI wafers [29]

There are two major steps in this process. The first one is the so called Silanol bonding technology also none as molecular or direct bonding. The goal of this technology is to bond to surfaces together. In our case, the LT with silicon oxide. The main steps of this technology are shown at figure 3.18.

The next step is the Smart-Cut technology, also invented by Soitec. The principle of the technology is based on ion implantation, by controlling the particle energy and flux, the depth of max implantation can be precisely controlled too. A thermal process is then applied and it yields to a progression of physical defects at this depth due to ion mobility and affinity. The implanted layer is thus separated from the rest of the wafer at the end of the process [28]. A high quality surface is then recovered thanks to a chemical-mechanical polishing (CMP).

Results from a study of Soitec which shows the interest and the quality of POI substrate are shown at Table 3.1 and 3.2 [30].

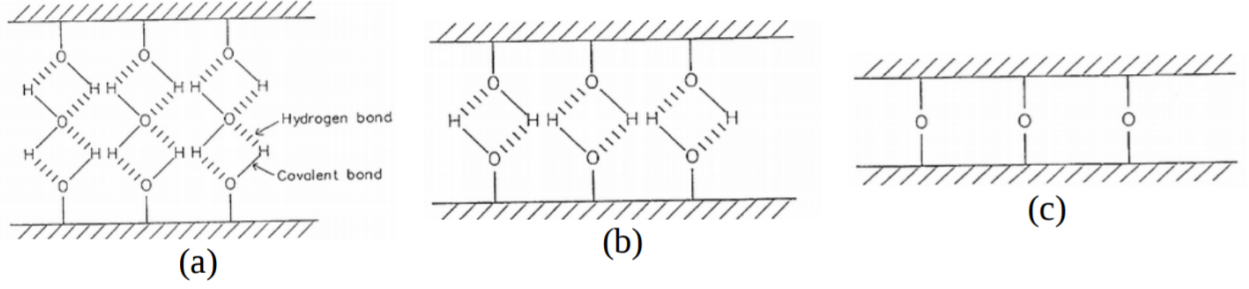


Figure 3.18: Main steps of Silanol bonding (from [12]) (a) hydrophilic association of surface mainly achieved with hydrogen bonds (b) partial drying of the interface to reinforce the bonding (c) total elimination of hydrogen bonds, covalent liaison between the surface (thermal process $> 1100^{\circ}\text{C}$) [28]

Trap Rich layer	None	Intermediate	Standard
Harmonic level - HD2 (dBm)	-40	-50	-85
Bode Q	271.8	495.9	1176.5

Table 3.1: Effect of trap rich layer [30]

	LT thickness (nm)	SiO ₂ thickness (nm)	Resonance frequency (MHz)
Mean Value	600	500	1867.1
Standard deviation	19.1	20.3	2.66

Table 3.2: Impact of the surface quality and uniformity on the resonance frequency [30]

Table 3.1 shows the impact of the trap rich layer which is a layer of polysilicon. The goal of this trap rich layer is to reduce substrate losses. POI substrate losses and linearity can be evaluated by Co Planar Wave guide (CPW) measurement of the fundamental and 2nd Harmonic (HD2) [30]. Furthermore, the quality factor is evaluated. The result is clear and the trap rich layer seems to reduce the electrical losses.

Table 3.2 shows the uniformity of LT and SiO₂ layer and the impact on resonance frequency. The thickness variation for both layers is in the order of magnitude of 20 nm. Such a variation leads to a standard deviation of the resonance frequency of 2.66 MHz.

3.5.3 Aluminium nitride

Aluminium nitride (AlN) is a famous piezoelectric material. It is even the first choice for resonator and sensors since AlN has a high power handling capability, has a good thermal stability and also offers a mature process which is complementary with CMOS technology [31]. Indeed thin film of AlN can be deposited with precise control of the thickness and uniformity with atomic layer deposition for example or with physical vapour deposition. Thanks to this properties, AlN is suitable for SAW, BAW and also Lamb wave resonators [32].

SAW resonators is the main topic of this thesis so we will focus on it. There are several type of AlN SAW resonator. IDTs can be deposited on a bulk AlN substrate [33] [34] or on a film of AlN which is deposited on a surface, such as AlN/Sapphire [35], AlN/Si [36] [37] [38], AlN/Pt/Si [39] [36], AlN/SiO₂/Si [40] [41] [37].

AlN SAW resonators are Rayleigh surface acoustic wave resonator. These Rayleigh wave are fast in aluminium nitride, around 5700 m/s [33]. It is more rapid than leaky wave in LT (≈ 4200 m/s). The resonance frequency in SAW is determined by the IDT period and velocity of the wave. A very fine lithography is often required to obtain high frequency range for resonators and filters. SAW resonators which used wave with higher speed can thus reach higher frequencies with the same level

of lithography accuracy. It can extend the upper limit of the applicable frequency range of SAW resonators [42].

Quality factors which can be obtained with different technologies using AlN in SAW devices can reach high values. Values can go from several hundreds (325 [35]) to value above thousand (1920 [43], 6380 [35]) depending on article and technologies.

The thermal coefficient of frequency (TCF) of AlN has been computed as -19 ppm/K [34] which is not that much, it is lower to the TCF of LiTaO₃ which is supposed to be between -30 and -40 ppm/K. It has been computed as -29.8 ppm/K and -36.6 ppm/K [27]. Furthermore the opposite temperature coefficients of delay of Si and AlN make these materials particularly suitable to implement thermally stable SAW devices [44]. AlN is thus suitable for temperature compensated SAW using Si and SiO₂. It is even possible to reach a TCF of zero by adjusting properly the thicknesses.

The effective electromechanical coupling factor is often the worst figure of merit for AlN SAW resonator and limit its use in wideband filters. Indeed the coupling factor of AlN is lower than 2% and often smaller than 1% (0.56% [35], 0.32% [38])

To increase the effective coupling factor, it is possible to dope AlN with Scandium (Sc). It will increase the AlN piezoelectric coefficient which directly impact the coupling factor [14]. It can increase the coupling factor by a factor 1.7 [31]. Indeed some article shows a effective coupling factor above 2% [45] by using scandium. Unfortunately doped AlN always come with a decrease of quality factor [14] [31]. Nevertheless, it can bring an increase of the FoM $Q \times k_{eff}^2$ until 50% [45]. Electromechanical coupling factor can also be larger for layered structure [42]. Indeed it can be design such as the SAW field concentrates on the piezoelectric film. The IDTs can then be placed properly for efficient SAW excitation.

Even it is not the main topic of this thesis, it seems relevant to mention that some good articles [31] [46] [47] present AlN resonators and filters using Lamb wave. These resonators are thin film of AlN, between two pairs of IDTs or between one pair of IDT and a floating electrode. These are free structure released after the fabrications. It combines the advantage of good properties of FBAR and the easiness to define the wavelength by lithography. Such kind of resonators and filters reach high performances. The phase velocity of this kind of wave is in the order of magnitude of 10 000 m/s, similar to the BAW, the quality factors are over thousand and some techniques are found to obtain high bandwidth opening capability dealing with the coupling factor of AlN resonator which is lower than 2%. They are promising solutions for 5G applications.

For our case, no specific design seems widely used today for AlN SAW resonator. Our goal here is to study an alternative technology to LT but study the configurations of AlN is out of the scope of this thesis. To have a proper comparison with SAW resonator on POI and on bulk LT, the simple configuration of SAW resonators built on AlN bulk substrate will thus be analyse here.

These wafers of AlN can be fabricated by hydride vapor phase epitaxy (HVPE) [48]. The principle is to grow a thick layer of AlN by HVPE on a silicon substrate. The substrate is then removed by chemical etching to obtain the AlN wafer. The thickness of these wafer can reach 1000µm.

Chapter 4

Method

In this section, we will explain the process we went through to simulate, fabricate and characterize our resonators.

4.1 Simulation

Simulations are useful as they make it possible to predict behaviors or results which we are supposed to observe. Comparisons of simulations and measurements also serve to validate the measurement methods and results. Indeed, if we observe the same result in both the simulations and the measurements, we can more easily conclude that the result is correct. Furthermore it allows to study the impact of things that cannot be tested materially. For example, resonators with small wavelengths are not possible to fabricate in good conditions as will be explained further. In our work, simulation also allows us to investigate resonators using aluminium nitride which is an interesting technology for SAW resonators. The scope of this thesis did not allow for the fabrication of such resonators, but simulations will be a good basis to discuss different resonator technologies.

Every simulation was performed using a COMSOL model. The first models which were built were 2D models then we moved on to 3D models which are closer to reality. The different models will be presented in this section.

4.1.1 Bulk lithium tantalate

4.1.1.1 2D

The first step of simulation is to create a model, which is defined by its geometry and the physical properties of the materials and their interface. As said previously, the first models built were 2D models. The simplest model, which is the 42°Y-X lithium tantalate (LT) LiTaO_3 bulk model, is presented here as an example to illustrate the possibilities of simulation. The model is shown at Figure 4.1a. It is composed of two electrodes of aluminium (with a thickness of $0.2\text{ }\mu\text{m}$) placed on the top surface of a substrate with a width of λ . The width of the electrodes and the spacing between electrodes is $\lambda/4$, as explained in section 3.4.2. The two electrodes represent one pair of fingers of the IDT: 1V is applied to one electrode, 0V on the other. The substrate is formed by a layer of piezoelectric material (LT in this case, with a thickness of 4λ) and a perfectly matched layer in the material of the bulk (in this case, also LT). The purpose of the perfectly matched layer is to mimic a non reflecting infinite domain. This layer is perfectly absorbing. This layer is there because the device we are simulating is in fact hundreds of micrometers thick. However, creating such a model on COMSOL would lead to a very high complexity, making simulation time much longer.

All of our models are composed of only a single pair of fingers for the same reason. It induces the fact that a periodic condition is imposed on the left and right side of the model. This simulates the repetition of a high number of the same structure on both sides of the model. It is important to remember that only one pair of IDT fingers is present in the model when comparing with measurements made on real-life resonators, which are of bigger scale. In addition to these physical

conditions, physical properties for each material are needed to define the model. They include electrical and mechanical properties, as well as electromechanical properties such as the piezoelectric constant. One key physical aspect is the modelling of losses. We previously presented the three kinds of losses in a piezoelectric resonator: mechanical, dielectric and coupling losses. Loss factors for those mechanisms can be introduced in COMSOL. Unfortunately, loss factors are really difficult to compute, and can be dependent on frequency. Only the dielectric loss factor ($\tan \delta$) was available in the literature [49] and was introduced in the model. It is worth mentioning that the model is meshed with the finest mesh provided by COMSOL which is the "extremely fine" mesh (shown at Figure 4.1b).

Once the model is built, several studies can be conducted in order to analyse the behavior of the

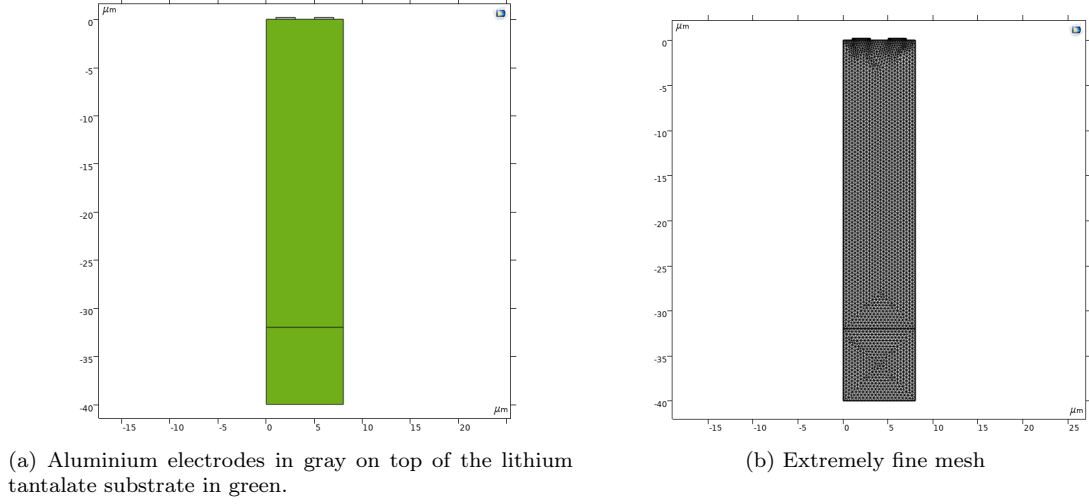


Figure 4.1: 2D model for COMSOL simulation, illustrated with the bulk LT model : 8 μm wavelength, two aluminium electrodes (0.2 μm thick), one layer of LT (4 wavelength thick), one perfectly matched layer of LT (1 wavelength thick).

model. The most relevant studies are the following :

- **Eigenfrequency study** : This study will give the resonance modes of the model. It is therefore relevant to look at the displacement of the model for the different resonance modes. Indeed only surface acoustic wave resonance modes are important in the context of SAW resonators. This is illustrated in Figure 4.2 which contains the plots of the displacement for a few resonances resulting from the eigenfrequency study.

In Figure 4.2 it is rather clear that the resonance modes of figures 4.2a and 4.2b correspond to surface acoustic waves (symmetric and anti-symmetric). However the other two resonance modes (Figure 4.2c and 4.2d) are examples of modes that do not correspond to surface acoustic waves and are thus irrelevant for this work.

- **Frequency domain study**: This study allows to simulate the reaction of the model with respect to frequency. Thanks to this study, some interesting graphs such as admittance or impedance curves are obtained and comparisons can be done with measurements and theoretical curves. From those graphs and the associated data, we can extract all relevant features such as resonance and antiresonance frequencies, lumped elements of the electrical model of the resonator and figures of merit. The extraction method is the same as with measurements and will be explained further in section 4.4.

The admittance curve is a typically interesting plot which is obtained with the frequency domain study, and is shown in Figure 4.3. The admittance is usually measured in Siemens, however Siemens is a valid unit for three-dimensional objects only. Because the model used here is in 2D, the correct units of the admittance would be Siemens per meter. In order to determine a value in Siemens, COMSOL makes the assumption that the model has a depth of 1 meter. It is important to keep this in mind when comparing 2D simulations with 3D simulations or real-life results.

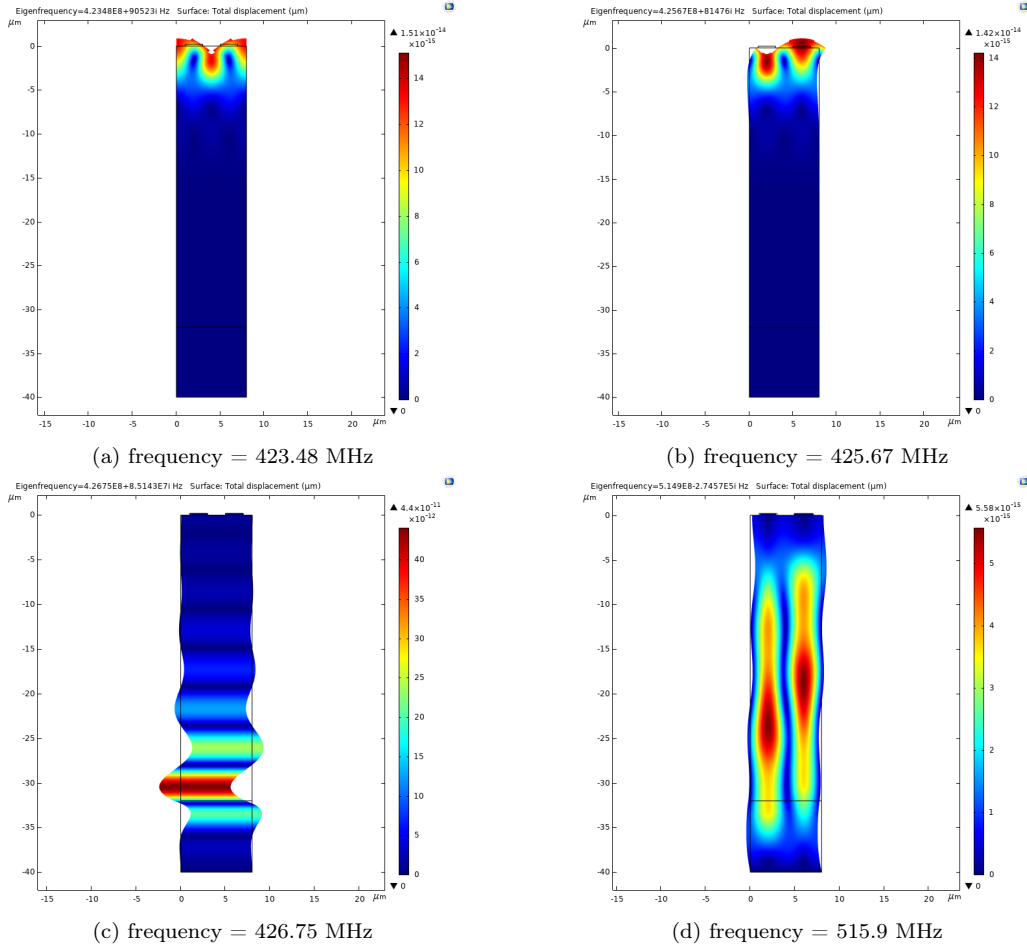


Figure 4.2: Eigenfrequency study results: displacement for different resonance modes

The resonance frequency observed on the admittance plot of Figure 4.3 is at 425.7 MHz which corresponds to the resonance mode of Figure 4.2b. The other resonance modes which are not SAW modes cannot be seen on the admittance plot because they do not influence the admittance. Indeed, as the electrodes are placed on the surface, modes that do not excite the surface of the substrate will not impact the electrodes and therefore their electrical response.

4.1.1.2 Evaluation of the simulation results

The admittance curve obtained by the simulation is very similar to the theoretical curve presented in Figure 3.6b of section 3.2. This is expected as the simulation is supposed to be almost perfect, with side effects and defaults omitted. If the model behaves as the theory suggests, we can conclude that it is valid.

Besides, the sharpness of the resonance and antiresonance in the admittance plot is a sign of good quality factor. The quality factor is directly dependent on the losses in the system, and is therefore influenced by the loss parameter input. The fact that some types of losses are not taken into account in the model might be the reason for this unexpectedly high quality factor. Another thing to notice is that the resonance and antiresonance are rather low compared to what we expect to observe. Indeed, as we saw previously, the speed of leaky SAWs in 42°Y-X lithium tantalate is around 4000 to 4200 m/s. In the simulation, we observe a speed of $425.7 \text{ [MHz]} \times 8 \text{ [}\mu\text{m]} = 3405.6 \text{ [m/s]}$ which is lower than expected. However, the orientation is supposed to be optimal in the simulation, and therefore should not be a reason for this attenuation. This can be explained by the fact that COMSOL does not consider the physical property tensors correctly when the model is in 2D, as they correspond to a 3D model. All those reasons prompted us to move to a 3D model in order to have more realistic

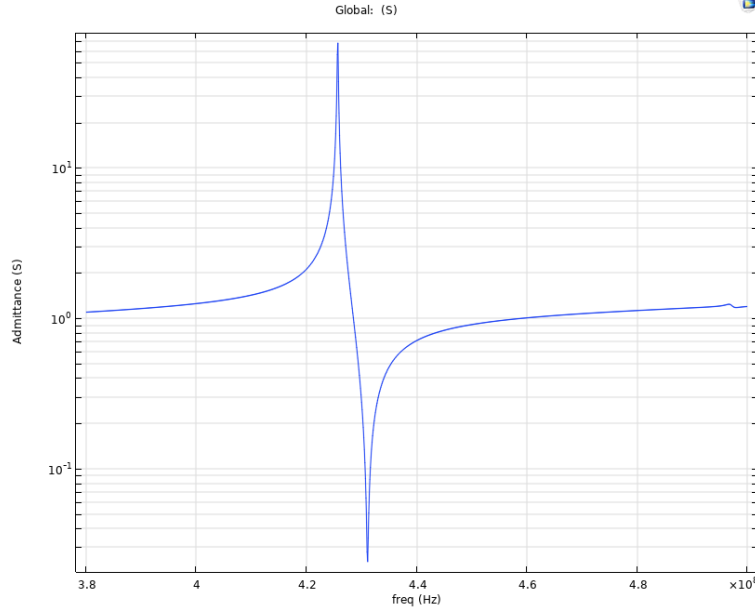


Figure 4.3: Admittance of the model for a simulation between 380MHz and 500MHz with a step of 100kHz.

simulations.

4.1.1.3 3D

3D models are closer to reality than 2D, but more complex and therefore require more computations, which makes the simulation time much longer. The 3D model for a bulk 42°Y-X LT resonator is shown in Figure 4.4. The dimensions (thickness and width) are the same as for the 2D model. Only the depth has to be added. The depth of the model is equal to the aperture width ($150\text{ }\mu\text{m}$ in the case illustrated in Figure 4.4). This time, the perfectly matched layer (PML) is not only under the substrate but also on the sides, at both ends of the electrodes. The width, depth and thickness of the perfectly matched layer are equal to the wavelength. As in 2D, there is a single pair of electrodes: one set at 1 V and the other at 0 V. No voltage is applied on the aluminium part of the perfectly matched layer.

Again, a single pair of IDT is modelled, and a periodic condition is imposed on both sides. As for the 2D model, dielectric losses are the only type of losses included in the model. The same studies as for the 2D model are conducted for the 3D model. Because the complexity of the 3D model is higher than that of the 2D model, the simulations are more complex and are longer. To keep simulation times reasonable, a trade-off has to be made and the choice of mesh is therefore limited. Indeed, if a fine mesh is chosen, simulations can take several hours, or even longer if the finer mesh is chosen. In our work, the mesh of 3D models will be specified when a simulation result is displayed. The different levels of mesh are compared in Figure 4.5.

- **Eigenfrequency study** : As seen previously (thanks to the 2D model), not all resonance modes are relevant to analyse for SAW resonators. This holds true for the 3D simulations. We will analyse the relevant resonance modes which correspond to surface acoustic waves. The plot of the displacement of the 3D model is available in Figure 4.6.

The simulation to obtain Figure 4.6 is done with a finer mesh. The resonance frequency is close to what we expect with the theory. A quick calculation can be performed : the speed of the surface acoustic wave in this simulation equals $505.47\text{ [MHz]}\times 8\text{ [}\mu\text{m]} = 4043.76\text{ [m/s]}$ which is in the expected range of values ($4000\text{--}4200\text{ m/s}$ for 42°Y-X LT, see section 3.5.1). The cross section view is very similar to the simulation in 2D, which also validates the model. A comparison can be done with other levels of mesh. The same plot for simulation with "fine" mesh and "normal" mesh are available in figures 4.7 and 4.8 respectively.

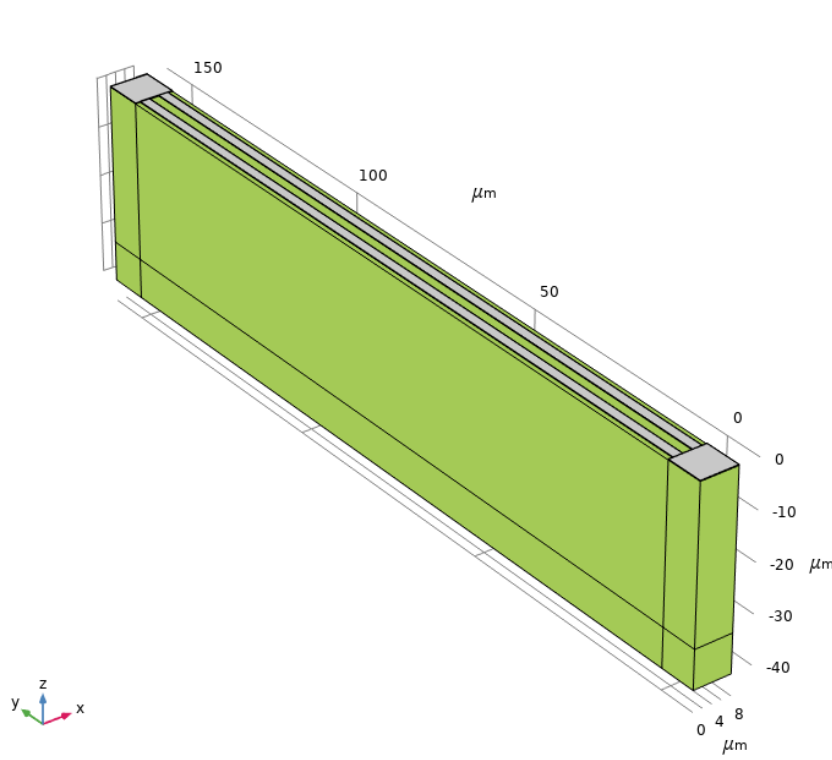


Figure 4.4: 3D model of the COMSOL simulation, illustrated for the bulk LT case: 8 μm wavelength, aperture width of 150 μm , two aluminium electrodes (0.2 μm thick), one layer of LT (4 wavelength thick). Aluminium is in grey, Lithium tantalate in green.

It is expected that the best result is obtained with the finest mesh. We can also conclude that the mesh has a significant importance in the simulation.

- **Frequency domain study :** As for the 2D simulation, this study allows for several valuable plots, including the admittance which will be analyzed here. The plot of the admittance for the 3 different meshes is available in Figure 4.9. It is clear that with increasingly fine meshes, the admittance plot becomes increasingly close to the theoretical curve. To correlate this graph to the eigenfrequency study results, the resonance that can be seen on the peak of the curve corresponds to the resonance observed during the eigenfrequency study.

While figures 4.9c and 4.3 show admittance curves similar to the theoretical curve both for 2D and 3D simulation, the value of the resonance frequency indicates that the 3D model is more realistic than the 2D model.

4.1.2 POI

This section will briefly describe the 2D and 3D models for the POI to make the simulations. The conclusion that the 3D model is more realistic than the 2D model is also true for the same reasons as for the resonator with a bulk of Lithium tantalate. No result will thus be shown in this section but only the presentation of the models.

The models in 2D and 3D are shown in figures 4.10a and 4.10b respectively (Figure 4.10c is a zoom of Figure 4.10b).

As for the bulk model there is a perfectly matched layer (PML) to mimic a non-reflecting infinite domain. The PML is at the bottom (for the 2D and 3D models), in front and behind the model (for

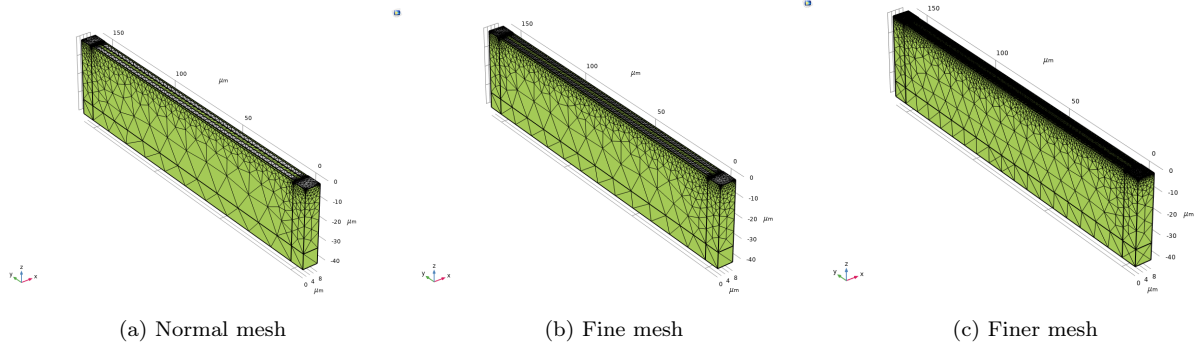


Figure 4.5: Comparison between meshes

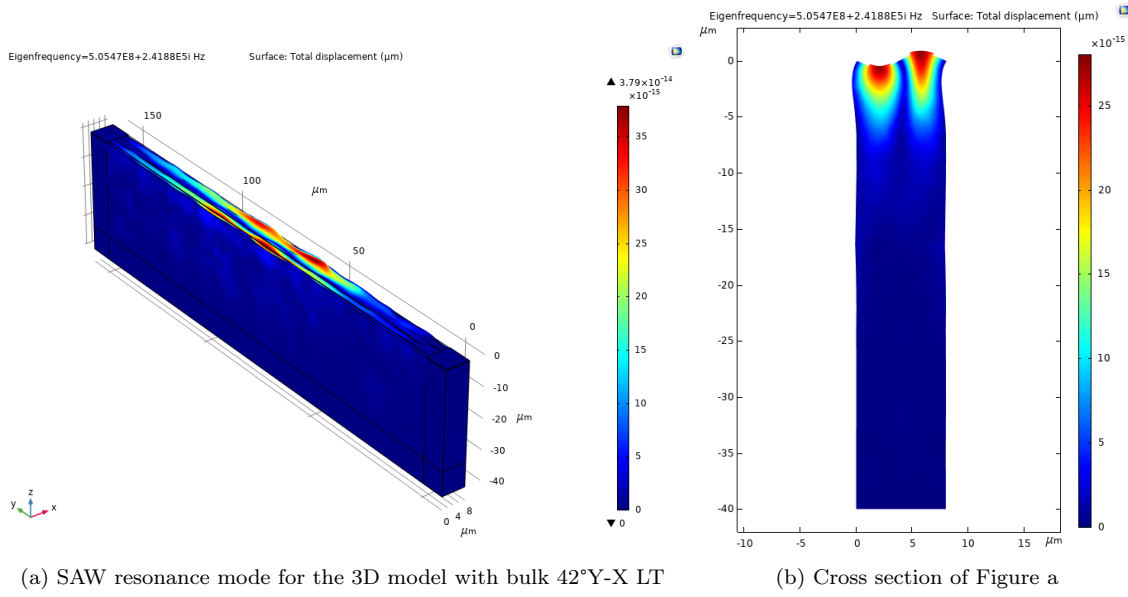


Figure 4.6: Displacement for the resonance mode at 505.47 MHz, simulated with a "finer" mesh

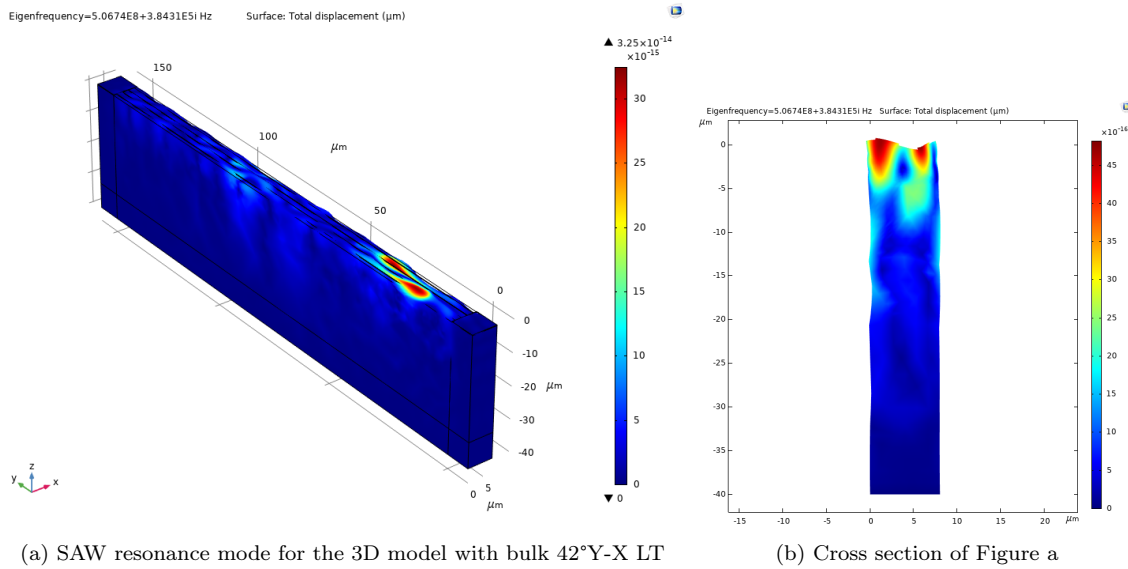


Figure 4.7: Displacement for the resonance mode at 505.47 MHz, simulated with a "fine" mesh

the 3D model only).

The conditions on the simulations are the same as for the bulk of lithium tantalate model. There is a periodic condition on the right and on the left sides to simulate the fact that there are a lot of

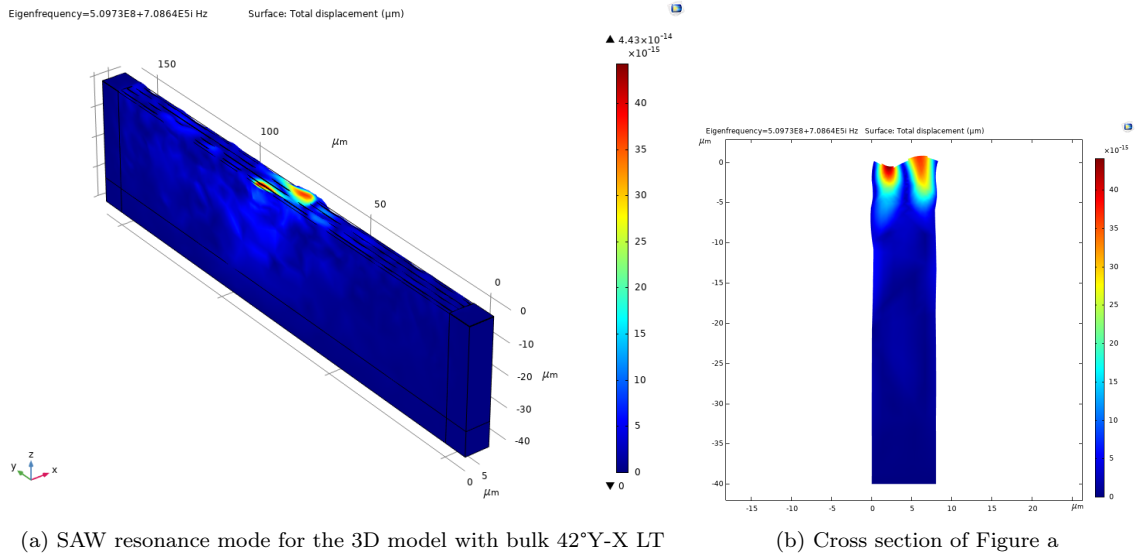


Figure 4.8: Displacement for the resonance mode at 505.47MHz, simulated with a "normal" mesh

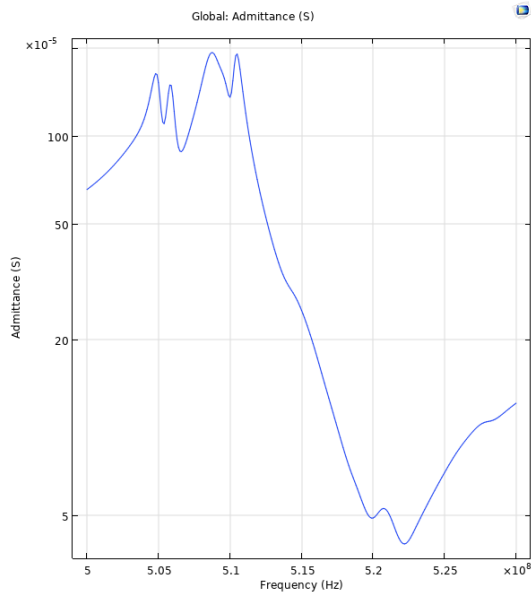
IDT fingers one next to the other. There is a fixed constraint at the bottom of the model (below the PML). One electrode is set at 0V and the other at 1V. A rotation of 42° is done to ensure the good crystal orientation of the model. As for the previous model, only the dielectric losses are introduced. The parameters used by COMSOL for the different materials are available in appendix D. The dimensions for the basic model of POI are the following :

- A wavelength of 8μm
- Width of electrodes equal to one quarter of wavelength spaced by one quarter of wavelength too
- Thickness of electrodes equal to 0.2μm
- Thickness of piezoelectric material equal to 0.6μm
- Thickness of oxide equal to 0.5μm
- Thickness of polysilicon (traprich layer) equal to 1μm
- Thickness of silicon substrate equal to four wavelengths
- Depth and thickness of PML equal to one wavelength
- Aperture width of 150μm (only for 3D model)

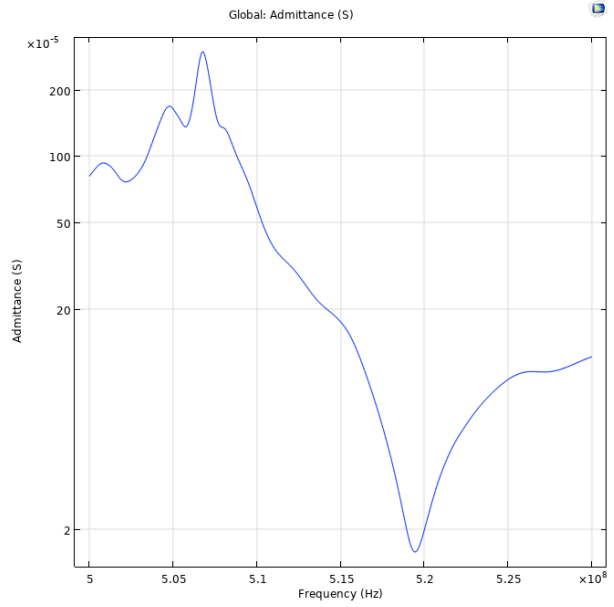
4.1.3 Aluminium nitride

The AlN COMSOL 3D model is shown at Figure 4.11.

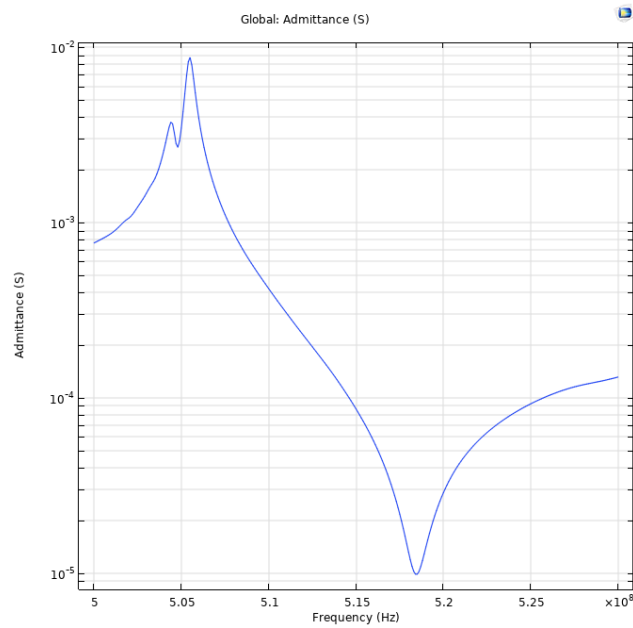
This model is exactly the same, with the same dimension, as the one built for bulk LT except the fact that lithium tantalate is replaced by aluminium nitride. The properties of both materials are shown in appendix.



(a) Admittance of the model with normal mesh

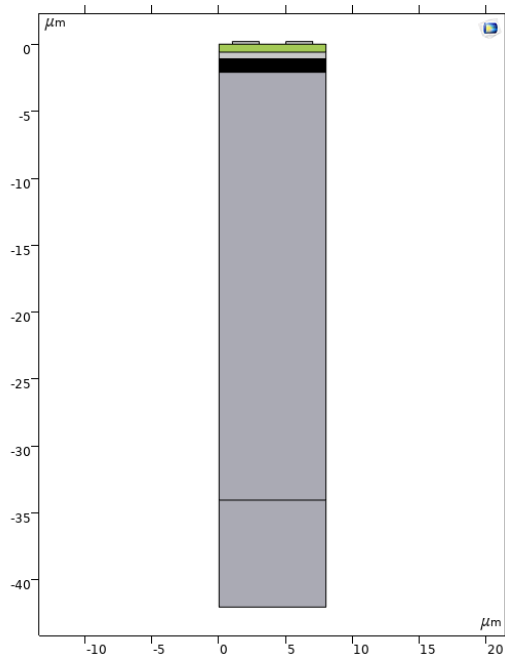


(b) Admittance of the model with fine mesh

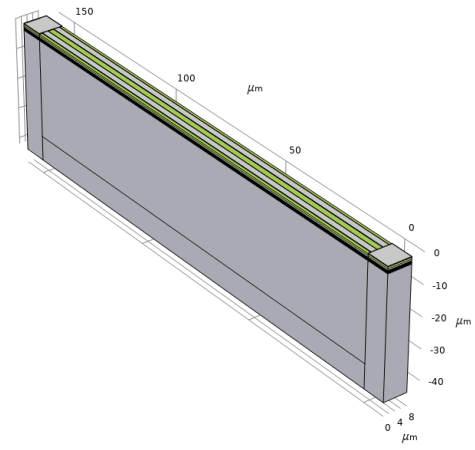


(c) Admittance of the model with finer mesh

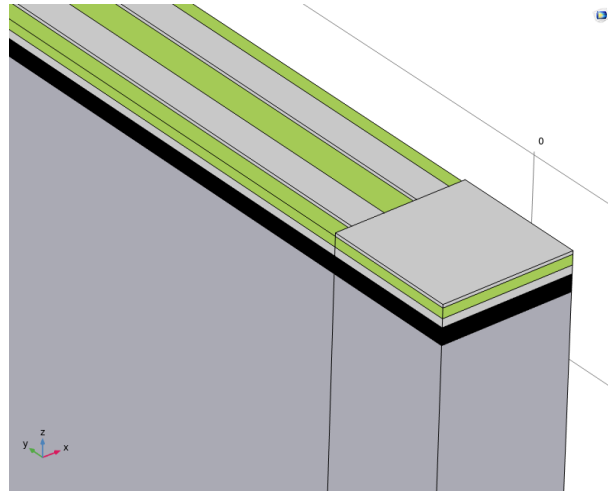
Figure 4.9: Plot of the admittance for simulations with different meshes. The frequency domain study is conducted from 500 MHz to 530 MHz with a step of 100 kHz



(a) 2D model



(b) 3D model



(c) 3D model zoomed

Figure 4.10: Model of the COMSOL simulation, illustrated for the POI: 8 μm wavelength, aperture width of 150 μm , two aluminium electrodes (0.2 μm thick), one layer of LT (0.6 μm thick), one layer of silicon oxide (0.5 μm thick), one layer of traprich (1 μm thick), one layer of silicon monocrystalline (4wavelength thick). Silicon is in grey, polysilicon is black, silicon oxide is light grey (between black and green layers). Lithium tantalate is in green, aluminium is in light grey on the top.

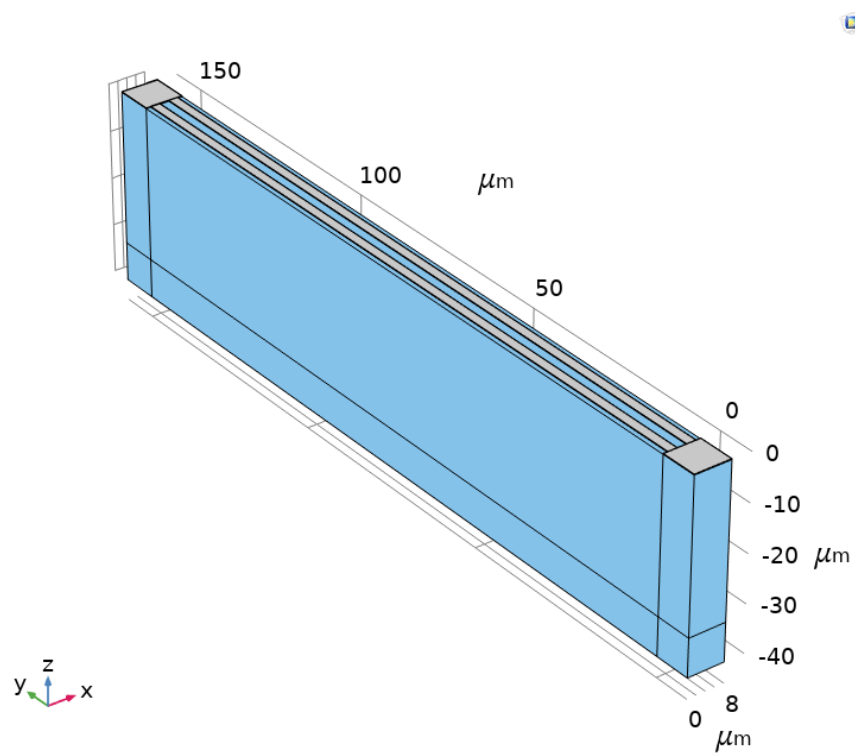


Figure 4.11: 3D COMSOL model for AlN technology

4.2 Fabrication

This section presents the design and fabrication of the resonators which have been used in our work.

4.2.1 Resonator design

The resonators we have used in our work have not been designed by us, but rather the mask design was provided by Incize, in the framework of the "CIVICS" project. The mask used to fabricate the resonators contains multiple repetitions of the same die, with the layout of this die detailed in appendix A. One such die contains 72 resonators, both single port and two ports, with several geometrical characteristics being varied. Those specifications are listed below and are illustrated in Figure 4.12, which shows a typical 2-port resonator such as those used in our work. The drawing used in the Figure is in fact part of the actual mask design file.

- Wavelength [μm] : this corresponds to the distance between two electrode fingers of the same voltage. It defines the resonance frequency of the resonator. In our work, possible values of wavelength are of 2, 8 and 16 μm .
- Aperture width [μm] : this is the distance between the tips of alternating electrodes. In other words, it is the distance fully covered by both sets of electrodes, and is therefore approximately the width over which the SAW can travel. Possible values in this design are 50 and 150 μm .
- Number of IDT fingers : this designates the number of fingers present on the IDT of one port of the resonator. Possible values in this design are 20 and 100.
- Number of mirror fingers : this designates the number of fingers present on one mirror (also called reflector) of the resonator. Possible values in this design are 10 and 100. Each resonator, whether 1- or 2-port, contains 2 mirrors placed at each side of the IDTs.
- Port spacing [μm] : this value is only relevant in the case of 2-port resonators, and is therefore omitted in the case of 1-port resonators. It simply designates the lateral spacing between the two ports. Possible values in this design are 16 and 160 μm .

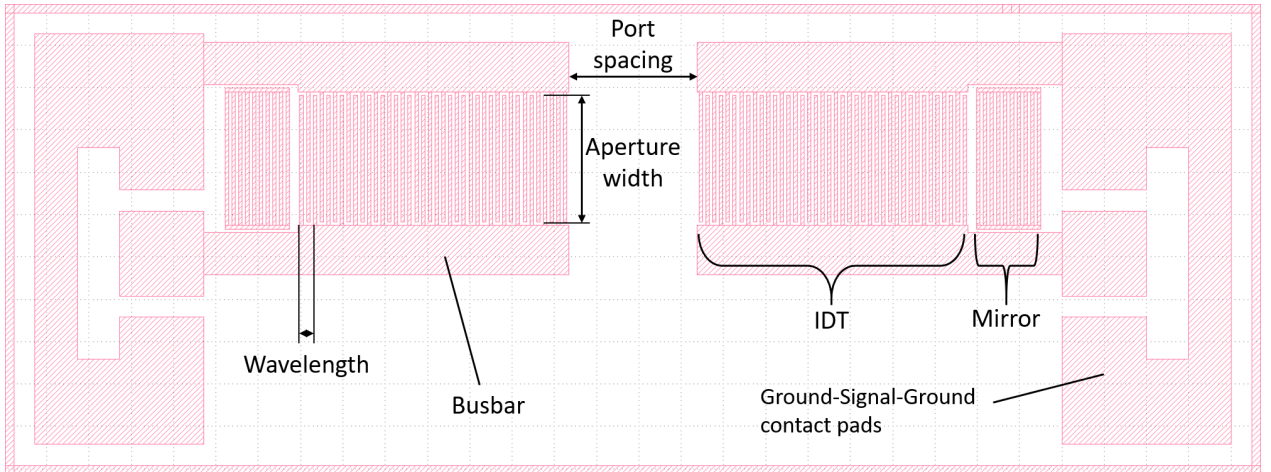


Figure 4.12: Schematic of a typical 2-port resonator, with key specifications highlighted.

In our work, not all resonators from the layout were used. Some resonators have been used predominantly, in order to serve as reference for various comparisons. Those resonators are presented in appendix A.4.

4.2.2 Pyroelectricity

Piezoelectric materials such as lithium tantalate are pyroelectric and ferroelectric (see section 3.3.3). Hence, they display pyroelectric effects. Although this can be beneficial in a number of applications,

in our work it is rather problematic for it causes issues during the fabrication process. Indeed, the accumulation of charges at the surface can cause electrical arcs to appear, which can fragilize the material. It is something we observed during our fabrication process. As it is likely the result of a sudden change in temperature, we adapted our process to produce smaller gradients of temperature. We based our improvements on advice from other scientists who had experienced the same kind of problem [50]. In practice, each time the wafer was put in hot temperatures (mainly in photoresist baking steps and dehydrating steps, occurring in ovens), we started by gradually heating the wafer on a hotplate, with a slow ramp up in temperatures. Similarly, when taking the wafer out of the oven, we held it in the air (under laminar flow to avoid unwanted particle deposition) for it to cool down, before being put in contact with colder surfaces. These additional precautions worked well and almost no electrical arc or spark was observed once these steps were put in place.

4.2.3 Process steps

The fabrication steps start from the wafer point. Bulk LiTaO_3 wafers have been provided by In-cize, while POI wafers have been provided by SOITEC. All the steps mentioned further have been performed in clean room in Winfab at UCLouvain. We have produced the resonators basing our process both on literature and on in-house expertise acquired by Winfab members over their years of working in microfabrication. Our fabrication process was modified and improved by trial and error as some aspects had not been taken into account initially. In total, we produced 4 wafers of resonators on bulk LiTaO_3 substrates, and one wafer of resonators on a POI substrate. The process step for the final bulk LiTaO_3 wafer and the POI wafer is detailed below. Other iterations of the process are described in appendix B.

1. Cleaning : the first mandatory step when handling wafers is to clean them to ensure no unwanted particles are present on its surface. Here, the lithium tantalate wafers were cleaned using a rather "soft" cleaning process of acetone and isopropanol (or methanol), then rinsing with water and drying with nitrogen. Hydrofluoric acid HF was avoided as we did not want to risk damaging the wafer surface.
2. Heating : in order to avoid any pyroelectric effect, the wafer was progressively heated on a heating plate, from room temperature to 110°C , with increments of approximately $10^\circ/\text{min}$.
3. Adhesion Promotion : this is performed in an LP-III vacuum oven ¹. In the oven, the water contained in the wafer is evaporated by a series of heated (120°C) evacuations and N_2 refills. Then hexamethyldisilazane (HMDS) flows into the evacuated chamber, forming a monolayer on the surface of the wafer that enhances the adhesion of the photoresist. This process is called HMDS vapor priming and takes about 20 minutes.
4. Cooling down : this is another step to avoid manifestations of pyroelectricity. Indeed, contact with the cold (room temperature) coating plate might induce a significant temperature gradient. The wafer was simply held at in the air under laminar flow (to avoid unwanted particle deposition) until it reaches room temperature.
5. Photoresist coating : photoresist was spin-coated in the Süss Gamma 80². AZ nLOF2020 resin was spun at 3000 rpm. It is a negative resin, which means that the exposed parts (with UV light) will become cross-linked and stable, and the unexposed part will be removed by a solvent developer. Negative resins are more suitable for lift-off because of their negative sidewall angles (see Figure 4.13).
6. Pre-exposure bake : this step evaporates the solvents present in the resin. The wafer was baked at 95°C for 90 seconds in the Süss Gamma 80 oven. Precaution is also taken here with regards

¹Winfab page : https://sites.uclouvain.be/winfab/NEW_website/Public/Facilities/Coating.php - Oven and hot plate part

²Winfab page : https://sites.uclouvain.be/winfab/NEW_website/Public/Facilities/Coating.php - Spin Coating part

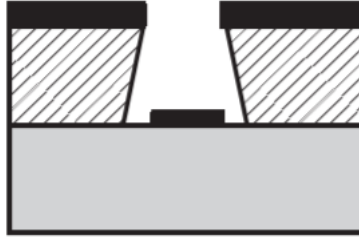


Figure 4.13: Substrate is in grey, negative resin is hatched, deposited layer to lift-off is in black [51]

to pyroelectricity : the oven has pins to hold the wafer in the oven, which then slide down to initiate contact between the wafer and the heating plate of the oven. To ensure gradual heating, the pins were maintained in the top position for a few minutes when the wafer is placed, before being put down.

7. Photolithography : During the photolithography, for a negative resin, the exposed area will cross-link and become insoluble. The lithography was performed in the Süss MA6 ³. Vacuum contact with the mask was used. Different exposure doses were tried by hiding some parts of the wafer. 60, 80, 100, 120, 140 and 160 mJ/cm² were used, with doses up to 100 mJ/cm² producing acceptable results, with the smaller doses yielding the best output.
8. Post-exposure bake : For some resists, the photolithography step only initiates the photopolymerization process and a post-exposure bake is needed to complete the process and generate the solubility difference between the exposed and unexposed part. After the photolithography, the wafer was thus baked again in the Süss Gamma 80 oven, this time at 110°C for 90 seconds. Again, a precautionary wait of a few minutes was performed when the wafer was placed on the pins, before allowing it to touch the heating part.
9. Cooling down : another step to avoid pyroelectricity. Indeed, contact with the cold (room temperature) development plate might induce a significant temperature gradient. The wafer was simply held in the air under laminar flow (to avoid unwanted particle deposition) until it reached room temperature.
10. Development : A solvent developer had to be used in our case due to the fact that we used a negative resin. The developer removes the resin parts which have not been cross-linked and rendered stable. It therefore dissolves the unexposed parts (as the resin is negative). 2 cl of developer (AZ 726 MIF) were poured on the wafer. After 60 seconds, the wafer was abundantly rinsed during at least another minute, then dried.
11. Metallization : a 200 nm thickness Al layer was then deposited by evaporation in the VST-TFDS 462 ⁴. The evaporation technique for the metallization is the most suitable technique for lift-off. Indeed, because of its poor step coverage, the sacrificial layer of resin will be etched easily by the acetone.
12. Lift-off : lift-off was performed in an acetone bath. Acetone selectively etches the resin against aluminium and silicon. Lift-off is enhanced with ultrasounds at 80 kHz to mechanically stimulate pieces of aluminium struggling to come off to remove them.

³Winfab page : https://sites.uclouvain.be/winfab/NEW_website/Public/Facilities/Lithography.php
 Manufacturer page : <https://www.suss.com/en/products-solutions/mask-aligner/ma-ba-gen4-series>

⁴Winfab page : https://sites.uclouvain.be/winfab/NEW_website/Public/Facilities/Deposition.php - PVD part
 Manufacturer page : <http://vacuumltd.com/#/products/evaporationSystemPage>

4.3 Model

The physical model used to describe our resonators is of utmost importance. The choice of model is a compromise between ease of computation and understanding of the underlying physics. A simple model offers very little insight into the physical mechanisms at play, but allows for repeatable, consistent extraction of numerical values, which in turn can be used for comparison purposes. On the other hand, additional model elements will make the extraction more error-prone, but offers more parameters to understand the origin of good or bad performances.

In this section, we are going to present and compare models with increasing complexity. Starting from the simple BVD model, we are successively going to add R_0 , R_s and L_s to end up with the complex mBVD model, which is the most complex one we will consider. We will then compare models based on both the values of lumped elements they give and the curve they produce when used to fit the experimental data of a reference resonator.

4.3.1 BVD model

The basic model for piezoelectric resonators is the Butterworth-Van Dyke (BVD) model (Figure 4.14), which is a lumped-element model for acoustic resonators such as SAW resonators. In this model, there are two parallel branches connecting ports 1 and 2. One branch accounts for the electrical behaviour and the other for the mechanical behaviour [14]. In the electrical behaviour branch, C_0 is the static capacitance, which is simply the capacitance between the IDT finger electrodes of the resonator [52]. This branch is also called the static branch. The mechanical (also called motional or dynamic) branch includes a motional resistance R_m , a motional capacitance C_m and a motional inductance L_m . The resonance of the resonator is the result of the series circuit $L_m - C_m$ which has a zero impedance at the resonance frequency (f_r), also called series frequency (f_s). The antiresonance of the resonator is due to the parallel circuit between L_m and C_m , and C_0 which has an infinite impedance at the antiresonance frequency (f_a), also called parallel frequency (f_p). The computation of these resonance and antiresonance frequencies is available in appendix C. This model is valid when the resonator is used at a frequency close to its resonance frequency [14].

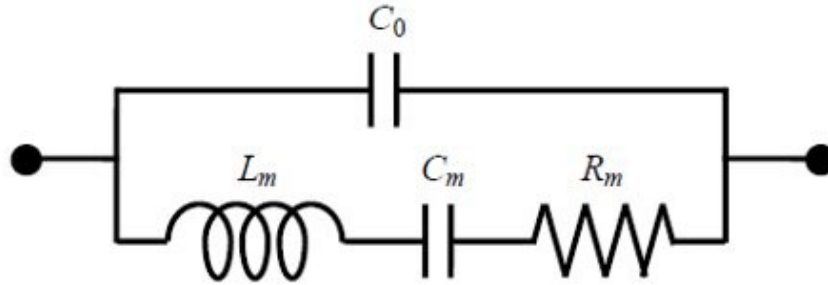


Figure 4.14: Butterworth-Van Dyke equivalent circuit [53]

4.3.2 mBVD model

In the modified BVD model (mBVD), resistances or inductances are added to account for ohmic and acoustic losses, and they improve the matching with the real piezoelectric resonator [52][1].

What we will usually refer to as "mBVD" model is the BVD model with two additional resistances: R_0 on the static branch which helps modelling dielectric losses and other loss mechanisms such as the acoustic leakage; and R_s in series with the rest of the circuit, which accounts for the resistance of the electrodes. These two elements, along with C_0 , constitute the static part of the circuit and will therefore be the only relevant elements far from the resonance. The mBVD model is pictured in Figure 4.16.

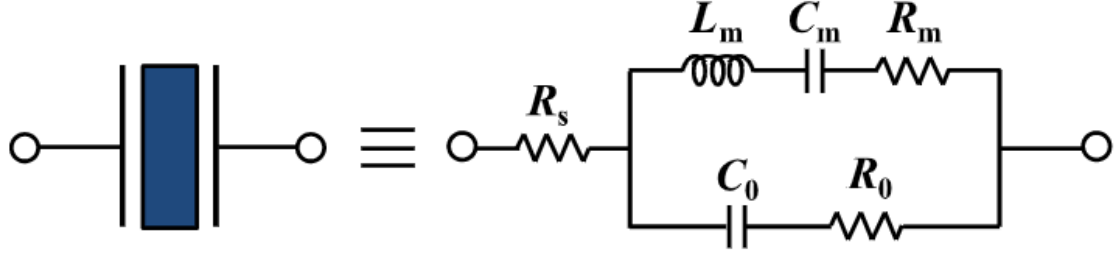


Figure 4.15: Modified Butterworth-Van Dyke (mBVD) equivalent circuit model for acoustic resonators [1]

4.3.3 Complex mBVD model

Further complexity is sometimes encountered in literature, as is the case with this modified version of the BVD model, that we will call "complex mBVD model" (Figure 4.16). This model includes an additional series inductance L_s accounting for unwanted series inductance caused by pads and wiring. This particular model also takes into account the contribution from the underlying oxide and Si substrate layers, but we will not consider them in our work. Indeed, this parallel part is supposed to be removed by the de-embedding as explained in section 4.4.4.

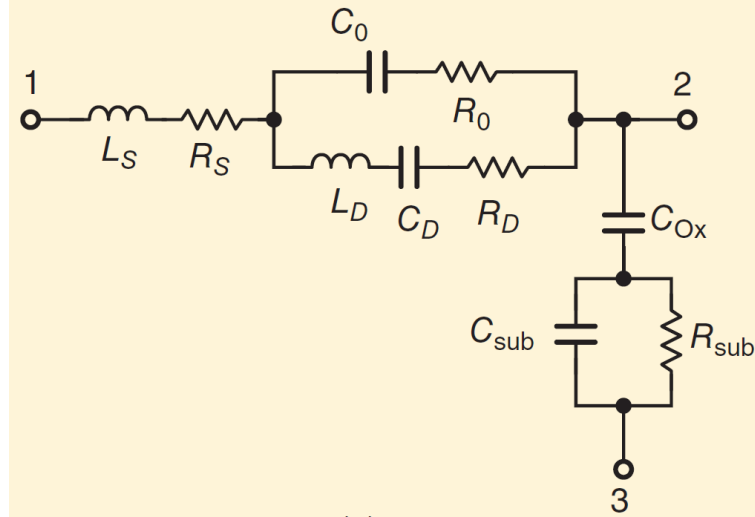


Figure 4.16: Complex mBVD equivalent circuit model for acoustic resonators [1]

4.4 Characterisation

4.4.1 Characterisation method and measurements

Characterisation is achieved using a Vector Network Analyzer (VNA), which yields S-parameters. The Network Analyzers are well known electrical machines able to measure the network parameters of an electrical network, typically our 1 or 2 port resonators. It commonly measures the S-parameter because reflection and transmission of electrical networks are easy to measure at high frequencies [54]. The name Vector Network Analyzer owes to the fact that it measures both amplitude and phase.

The VNA used for the measurements is a VNA with a frequency range between 5Hz and 3GHz. The probes which connect the VNA to the resonator are probes with 3 pins Ground-Signal-Ground. This is the reason why there are three connections on the frame of the resonators. A calibration is performed before each measurement. There are four steps to the calibration. Three for the reflection: Open, Short, Load (with a load of $50\ \Omega$), and one for the transmission (called Through) between the probes.

4.4.2 S-parameters

The S-parameters or scattering parameters, measured thanks to the VNA, can be written in matrix form. Here is the matrix form for a two-port network :

$$S = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix}$$

S-parameters are often used when we work with RF because the power at these frequencies is easier to quantify than the current or the voltage. Indeed, the different elements of matrix S are ratios of power. A two-port network will be used for the explanation, but it can be generalized for bigger networks. The S-parameter matrix is defined as follows :

$$\begin{pmatrix} b_1 \\ b_2 \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$$

With a_i and b_i respectively the incident and reflected power waves at port i as shown in Figure 4.17. The different elements of the S-parameter matrix are defined as :

$$S_{ij} = \frac{b_i}{a_j} \Big|_{a_k=0 \text{ for } k \neq j} \quad (4.1)$$

For a 2-port network, we have :

$$\begin{aligned} S_{11} &= \frac{b_1}{a_1} \Big|_{a_2=0} \\ S_{12} &= \frac{b_1}{a_2} \Big|_{a_1=0} \\ S_{21} &= \frac{b_2}{a_1} \Big|_{a_2=0} \\ S_{22} &= \frac{b_2}{a_2} \Big|_{a_1=0} \end{aligned} \quad (4.2)$$



Figure 4.17: S-parameter schematic [55]

4.4.3 Y-parameters and Z-parameters

We can convert S-parameters into admittance parameters, also called Y-parameters, through the following transformations [55] :

$$\begin{aligned} Y_{11} &= \frac{((1 - S_{11})(1 + S_{22}) + S_{12}S_{21})}{\Delta S_Y} Y_0 \\ Y_{12} &= \frac{-2S_{12}}{\Delta S_Y} Y_0 \\ Y_{21} &= \frac{-2S_{21}}{\Delta S_Y} Y_0 \\ Y_{22} &= \frac{((1 + S_{11})(1 - S_{22}) + S_{12}S_{21})}{\Delta S_Y} Y_0 \end{aligned} \quad (4.3)$$

where

- $\Delta S_Y = (1 + S_{11})(1 + S_{22}) - S_{12}S_{21}$

- Y_0 is the characteristic admittance which is assumed to be the same for the two ports. In our case, it is taken as $Y_0 = \frac{1}{Z_0} = \frac{1}{50} [\text{S}]$, as Z_0 , the characteristic impedance, is assumed to be 50Ω .

The reverse transformation is also useful [56] :

$$\begin{aligned} S_{11} &= \frac{(1 - Z_0 Y_{11})(1 + Z_0 Y_{22}) + Z_0^2 Y_{12} Y_{21}}{\Delta} \\ S_{12} &= \frac{-2Z_0 Y_{12}}{\Delta} \\ S_{21} &= \frac{-2Z_0 Y_{21}}{\Delta} \\ S_{22} &= \frac{(1 + Z_0 Y_{11})(1 - Z_0 Y_{22}) + Z_0^2 Y_{12} Y_{21}}{\Delta} \end{aligned} \quad (4.4)$$

with

$$\Delta = (1 + Z_0 Y_{11})(1 + Z_0 Y_{22}) - Z_0^2 Y_{12} Y_{21}$$

Finally, it also helps to convert S-parameters into Z-parameters, which are impedance parameters, using the following transformation [57] :

$$\begin{aligned} Z_{11} &= \frac{((1 + S_{11})(1 - S_{22}) + S_{12} S_{21})}{\Delta S_Z} Z_0 \\ Z_{12} &= \frac{2S_{12}}{\Delta S_Z} Z_0 \\ Z_{21} &= \frac{2S_{21}}{\Delta S_Z} Z_0 \\ Z_{22} &= \frac{((1 - S_{11})(1 + S_{22}) + S_{12} S_{21})}{\Delta S_Z} Z_0 \end{aligned} \quad (4.5)$$

where

- $\Delta S_Z = (1 - S_{11})(1 - S_{22}) - S_{12} S_{21}$
- Z_0 is the characteristic impedance equal to 50Ω .

4.4.4 De-embedding

De-embedding is a post-measurement process used to remove the parasitic elements taken into account in the measurements and minimize errors. Indeed, when we characterize devices under test (DUT), sometimes we need to add a "frame" between the probes and the device in order to make the measurements properly. In our case, this frame is made of contact pads and bus bars, indicated on the schematic of a resonator in Figure 4.12. The DUT is then called an embedded DUT. De-embedding is mathematically removing the measurements affected by the frame, leaving only the behavior of the device under test. This is commonly used when there are non-coaxial connections from the VNA to the DUT [58], which is the case with our devices. A de-embedding method is used to isolate the behavior of the resonator itself.

The de-embedding technique used in this case is called the open de-embedding (OPD) [59], it is widely used because of its simplicity. Indeed, the only thing needed to perform the de-embedding is the frame without the DUT, in our case it is just a set of pads without IDTs. This method assumes that the parasitics leading to the DUT are parallel admittances. The principle is shown at Figure 4.18 for a two-port DUT. In Figure 4.18(a), the equivalent circuit of the embedded DUT is shown. Figure (b) shows the equivalent of the open circuit with only the parallel admittances. Figure (c) shows the equivalent circuit when the DUT is short-circuited. The following computation is performed to isolate the admittance of the DUT:

$$Y_{DUT} = [(Y_{Measurement} - Y_{Open})^{-1} - (Y_{Short} - Y_{Open})^{-1}]^{-1} \quad (4.6)$$

This equation can be simplified if the impedance Z_{L1} is assumed negligible (≈ 0). Then the equation becomes :

$$Y_{DUT} = Y_{Measurement} - Y_{Open} \quad (4.7)$$

This computation must be done for every frequency step. Hence the measurements of the "open" must be done for the same frequency range and the same step that those of the DUT.

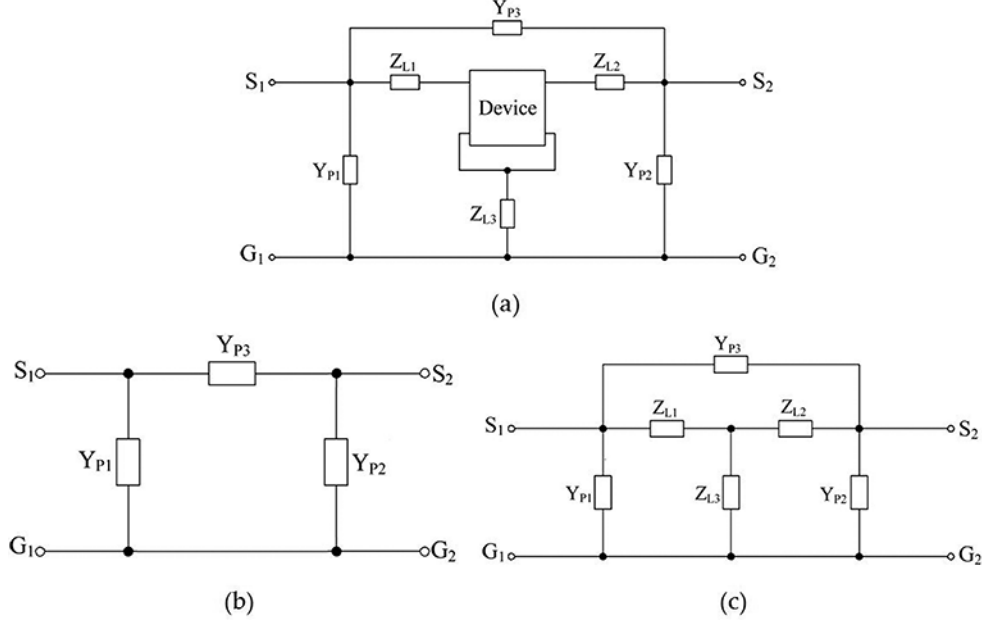


Figure 4.18: Equivalent circuit for (a) embedded DUT (b) open circuit (c) short circuit [60]

After de-embedding we are supposed to have a correct version of the Y-parameters. We then have to reconvert these Y-parameters to S or Z-parameters if those parameters are needed.

In our case we do not have de-embedding structure on the mask. Nevertheless, some structures are done to build resonators with a wavelength of 2 microns, so fingers of 500nm. Unfortunately these structures are often too precise for the lift process especially on a exotic substrate as LT. The result is that a lot of resonators are just open structures which can be used to deembed. Furthermore, due to bad exposure time (too long or too short), some structure, even larger than 2microns wavelength are just open structure. Pictures of these resonators are available in the appendix E.

4.4.5 Parameter extraction

Now that the BVD and mBVD models have been introduced, we can use these models to extract the parameter values of the equivalent circuit. We will then be able to use these parameters to compare and evaluate different resonators.

A typical extraction of different models and a comparison between these models is shown in appendix F

4.4.5.1 Resonance and antiresonance frequencies

Resonance and antiresonance frequencies can be found by 2 methods. The first one is to take the frequency where admittance is the highest for resonance and the lowest for antiresonance as shown in Figure 3.6b for example.

The second way to find them is to look at the phase. The response of piezoelectric resonators is capacitive far from resonance (dominated by C_0), inductive between resonance and antiresonance and the response is purely resistive at resonance and antiresonance. The phase during resonance and antiresonance is thus equal to zero. It is shown at Figure 4.19.

This second method is chosen in this thesis. It avoid some mistakes when wide range are taken and when a lot of some noise affect the admittance in measurements.

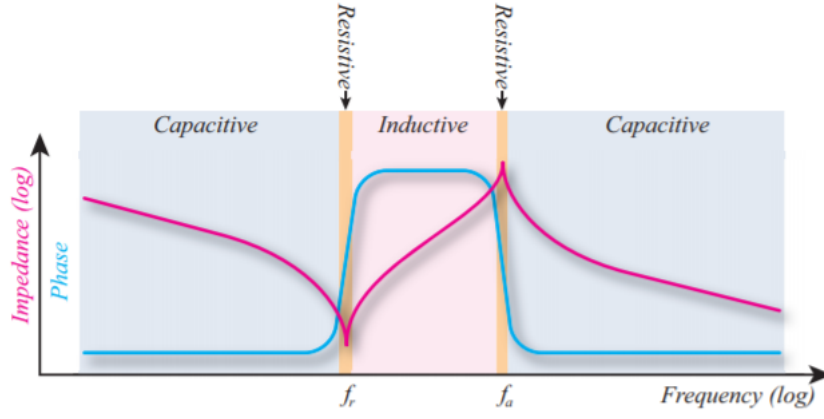


Figure 4.19: Impedance and phase of impedance of a piezoelectric resonators versus frequency [61]

4.4.5.2 Quality factor

The Q factor or quality factor is one of the main figures of merit that we will extract from our resonators. It is a dimensionless parameter that indicates the energy losses within a resonant element [62]. An increase in the Q factor means a decrease of the losses. The quality factor as a measure of the damping and as a Figure of merit for the resonators is already described in sections 3.3.2.2 and 3.4.4 respectively. A higher value of Q also corresponds to a more narrow, sharper bandwidth of the filter which is useful to remove the spurious signals [62].

Several methods exist to compute the quality factor of SAW resonators. Four different techniques are explained in this section [42]. Each technique presented here aims to find the quality factor at resonance frequency.

The first method supposes a correct extraction of the lumped elements of the BVD model. The computation to find the quality factor is shown in equation (4.8).

$$Q_r = \frac{\omega_r L_m}{R_m} = \frac{1}{\omega_r C_m R_m} \quad (4.8)$$

Where L_m , C_m and R_m are respectively the motional inductance, the motional capacitance and the motional resistance. ω_r is the angular resonance frequency (rad/s) equal to $2\pi f_r$ (f_r being the resonance frequency in [Hz]).

The second and third methods are based on the same principle. On one hand the conductance (G , which is the real part of the admittance) is used while on the other hand the magnitude of the admittance ($|Y|$) is used. The formula is shown at equation (4.9).

$$Q_r = \frac{\omega_r}{2\delta\omega} = \frac{f_r}{2\delta f} \quad (4.9)$$

For the method with the conductance, $2\delta\omega$ is the width of the conductance plot at half the maximum conductance. For the method with the admittance, $2\delta\omega$ is the width of the admittance plot at $|Y| = \frac{|Y_{max}|}{\sqrt{2}}$. These 2 methods are shown in Figure 4.20.

The last method is based on the derivative of the phase of the admittance. An illustration of the graph of the derivative of the admittance is shown at Figure 4.21. The formula used to compute the Q factor for this method is available in equation 4.10.

$$Q_r = -0.5\omega_r \frac{d\phi}{d\omega} = -0.5f_r \frac{d\phi}{df} \quad (4.10)$$

Where ϕ is the phase of the admittance.

The method which is chosen to compute the quality factor in this thesis is the last method (equation (4.10) and Figure 4.21). The first method depend on lumped element which are also

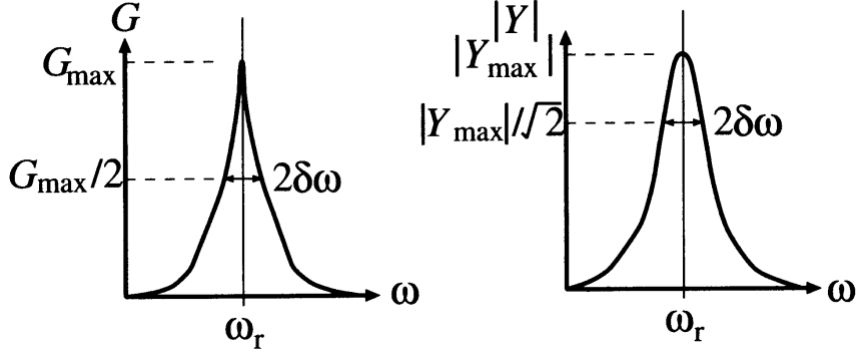


Figure 4.20: 2nd and 3rd method for the computation of the quality factor based on conductance and admittance respectively [42]

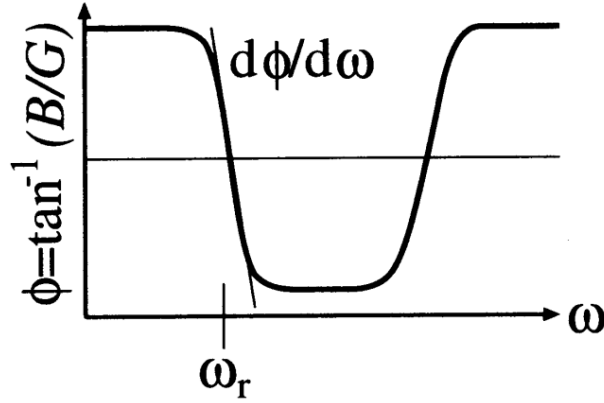


Figure 4.21: Illustration of the phase of the admittance [42]

extracted from measurements. This is thus a source of errors if lumped element are inexact. Then the second method require to know precisely the resonance frequency in order to find $|Y_{max}|$, $|Y_{max}|/\sqrt{2}$ and then the width $2\delta\omega$ (same principle with conductance). This method is strongly dependent on the value of the resonance frequency, so the step too. Third method is chosen because it is more direct and robust.

4.4.5.3 C_0

The static capacitance C_0 is simply the capacitance between the electrode fingers of the IDT in the resonator. It can be identified by fitting the admittance plot far from the resonance [1] (Figure 4.22). However, it should be noted that this method can still produce some fluctuations in the results as it depends on the range of frequency chosen to fit the curve. Figure 4.23 shows how we fitted the admittance (blue curve) to find C_0 (red line, which corresponds to $2\pi f C_0$) for one of our resonators. It is easy to see that the more frequencies close to the resonance we take into account, the higher the red line (fitted line) will be. Here, we have used the first 800 points, which corresponds to frequencies ranging from 1MHz to 150 MHz, while the resonance is at around 250MHz.

4.4.5.4 R_{stat} ($R_0 + R_s$)

This stage is only necessary for the extraction of the mBVD components. We define R_{stat} (for static) as the sum of R_0 and R_s . Far from the resonance, only the static part of the equivalent circuit (C_0 , R_0 , R_s) remains relevant in the electrical response of the resonator. Therefore, we can find R_{stat} by fitting the real part of the impedance Z far from the resonance.

$$R_{stat} = R_0 + R_s \quad (4.11)$$

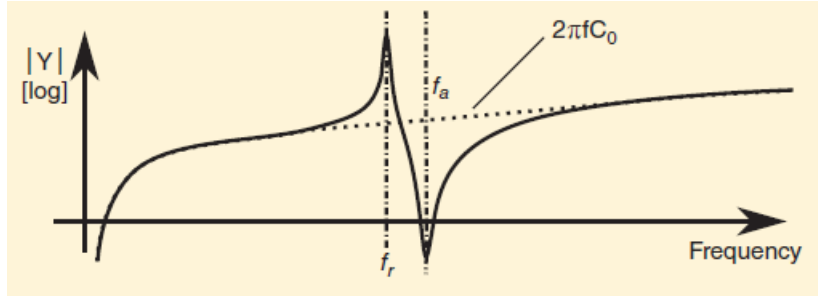


Figure 4.22: Identification of C_0 from the admittance plot [1]

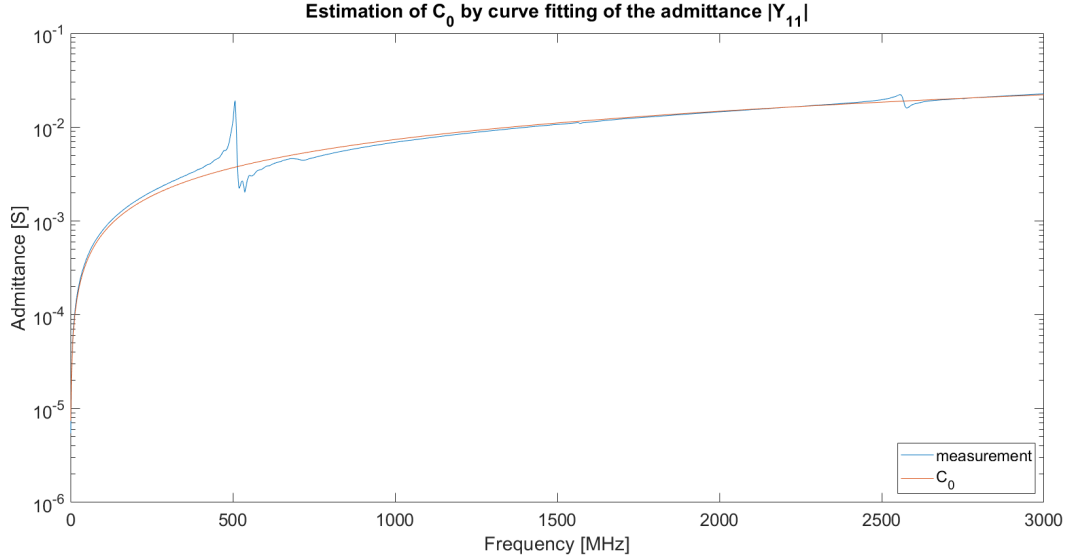


Figure 4.23: Fitting of the admittance curve of the measurements to extract C_0

Indeed, it seems normal that the real part of the impedance far from the resonance is almost equal to $R_0 + R_s$ when looking at the equivalent circuit of Figure 4.16. In order to show it properly we can find the impedance of the mBVD model which is calculated as follows:

$$Z_{mBVD} = R_s + \frac{(R_0 + \frac{1}{j\omega C_0})(R_m + \frac{1}{j\omega C_m} + j\omega L_m)}{R_0 + \frac{1}{j\omega C_0} + R_m + \frac{1}{j\omega C_m} + j\omega L_m} \quad (4.12)$$

When we plot the real part of the impedance of the mBVD model and compare it with R_{stat} , we find the plot at Figure 4.24. The different values were chosen arbitrarily in the order of magnitude of the measurements.

Figure 4.25 shows the application of the real part of the impedance curve fitting. The data comes from our measurements. <https://fr.overleaf.com/project/607405f3f977bab2201b5bbb> We can observe that we obtain a negative value for R_{stat} , which is of course not physically possible. This might be explained by the fact that no de-embedding was applied on this data. De-embedding might correct some errors.

4.4.5.5 C_m and L_m

The motional capacitance and inductance are linked to the resonance frequency and anti-resonance frequency [1].

$$f_r = \frac{1}{2\pi\sqrt{C_m L_m}}$$

$$f_a = \frac{1}{2\pi\sqrt{L_m \frac{C_0 C_m}{C_0 + C_m}}}$$

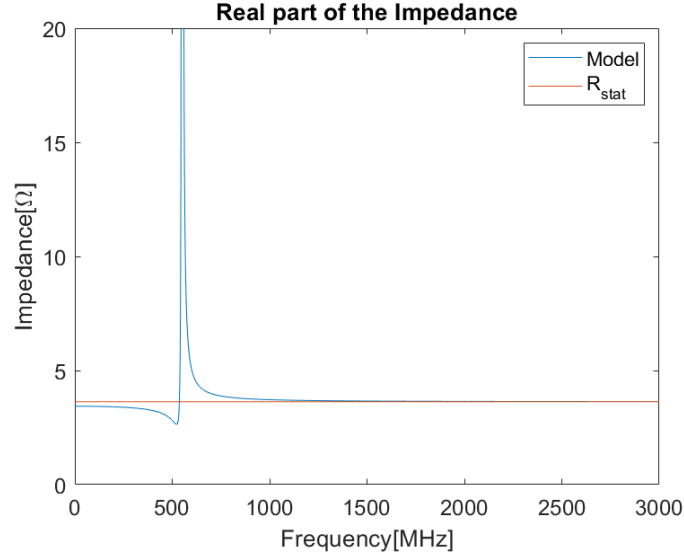


Figure 4.24: Comparison between R_{stat} and the real part of Z_{mBVD}

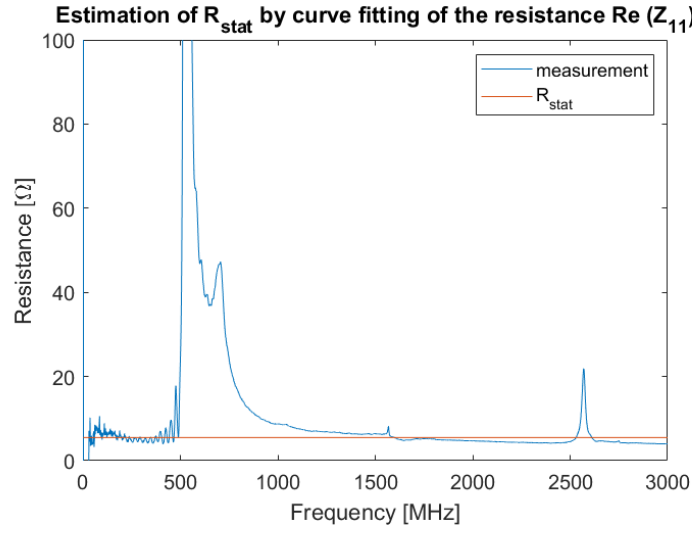


Figure 4.25: Comparison between R_{stat} and the real part of Z_{11} from the measurements

Re-arranging these equations gives :

$$C_m = C_0 \left(\frac{f_a}{f_r} - 1 \right)$$

$$L_m = \frac{1}{C_m (2\pi f_r)^2}$$

4.4.5.6 R_m, R_0, R_s

mBVD model :

R_m, R_0 and R_s are linked to the quality factors at the resonance (Q_r) and at the anti-resonance (Q_a) as follows :

$$Q_r = \frac{1}{\omega_r (R_m + R_s) C_m} \quad (4.13)$$

$$Q_a = \frac{1}{\omega_a (R_m + R_0) C_m} \quad (4.14)$$

where :

- ω_r is the angular resonance frequency
- ω_a is the angular anti-resonance frequency
- Q_r is the quality factor at the resonance frequency, calculated with equation (4.10) :

$$Q_r = -0.5\omega_r \frac{d\phi}{d\omega} \Big|_{\omega=\omega_r}$$

- Q_a is the quality factor at the anti-resonance frequency, calculated with equation (4.10) :

$$Q_a = 0.5\omega_a \frac{d\phi}{d\omega} \Big|_{\omega=\omega_a}$$

Using equations (4.13),(4.14) and the definition of R_{stat} (4.11), we can determine the values of R_m , R_0 and R_s .

BVD model :

In the case of the simple BVD model, only R_m needs to be found. In that case there are two ways to find R_m .

The first one is to use the formula of the quality factor described in equation (4.8) :

$$Q_r = \frac{\omega_r L_m}{R_m} = \frac{1}{\omega_r C_m R_m}$$

Re-arranging this equation, R_m can be found as shown in equation (4.15).

$$R_m = \frac{\omega_r L_m}{Q_r} = \frac{1}{\omega_r C_m Q_r} \quad (4.15)$$

With L_m , C_m found as in section 4.4.5.5 and Q_r found as in section 4.4.5.2.

The second method is to take the inverse of the conductance at the resonance frequency.

$$R_m = G^{-1}|_{f=f_r} \quad (4.16)$$

Indeed at the resonance frequency, the series circuit $L_m - C_m$ is short-circuited. In Figure 4.14 the only things remaining are R_m in parallel with C_0 . The conductance is then simply $\frac{1}{R_m}$.

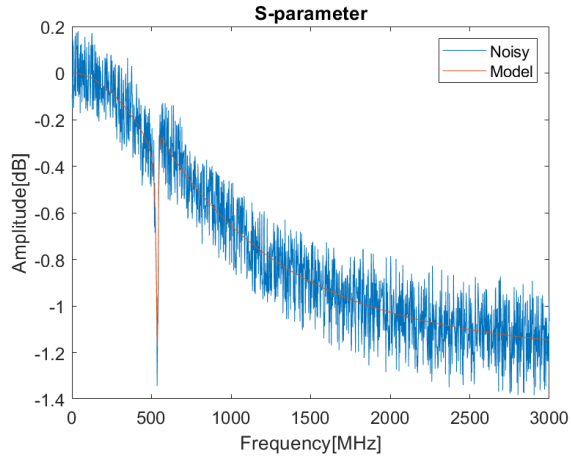
4.4.5.7 Impact of noise

Noise can impact the extraction of measurements. To modelize it we took an mBVD model (extracted from resonator 4, POI) with its lumped element. Once the model was built a conversion from Z-parameter (impedance) to S-parameter has been done. A noise was add to this S-parameter to simulate some noise during measurements. The S-parameter and noisy S-parameter are available in Figure 4.26a and the difference between both curves is shown in Figure 4.26b.

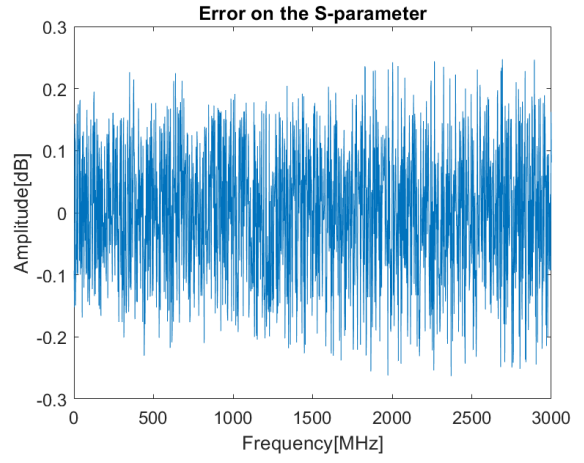
The noise on S-parameter is here uniform.

From this noisy S-parameter, the admittance which is used to find C_0 can be found. The Y-parameter (admittance) which comes from the noisy S-parameter and the admittance of mBVD model are shown in Figure 4.27a and the difference between both curves is available at Figure 4.27b. This time, the amount of noise increase when the admittance increase. There is a peak at resonance which is difficult to see on Figure 4.27a as the value of the noise is small compare to the value of the admittance. The noise is also more important on the right part of the graph. The way to find C_0 is to fit a curve of the first order and to find C_0 thanks to the slope. This means that took only the last point of the curve is a bad idea because the slope can be more biased due to the noise.

The same thing can be analysed for the real part of the impedance from which $R_{stat} = R_0 + R_s$ is determined. Once more the plot of the noisy curve and the curve of the model is plot in Figure 4.28a while the difference between both curve is plot in Figure 4.28b. The opposite occurs this time because the error is bigger at low frequency. As R_{stat} is obtained by fitting this curve with a constant, the less noisy part will give us the best result. The high frequency range far from resonance is thus more reliable.

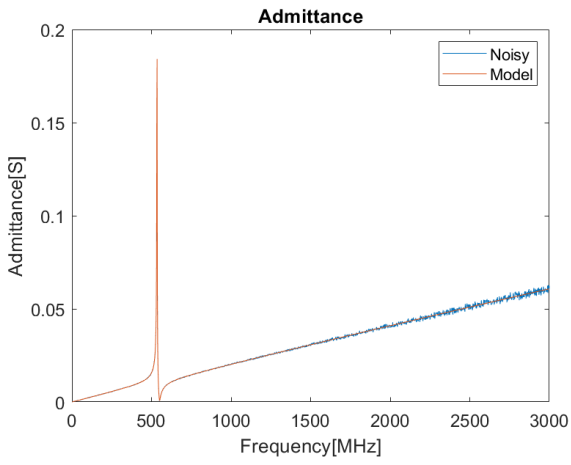


(a)

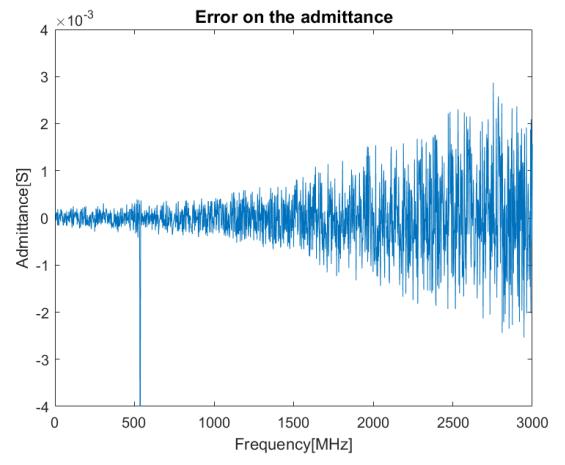


(b) Cross section of Figure a

Figure 4.26

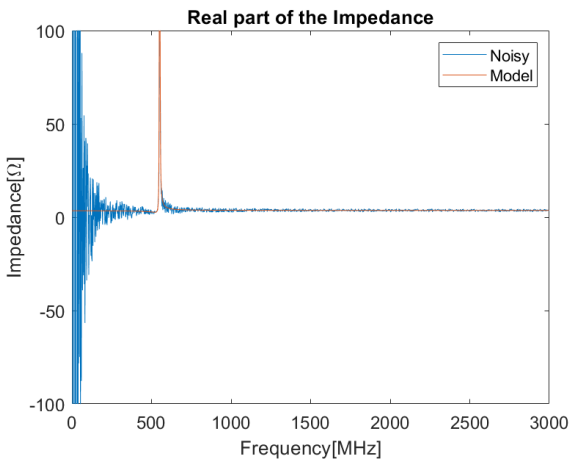


(a)

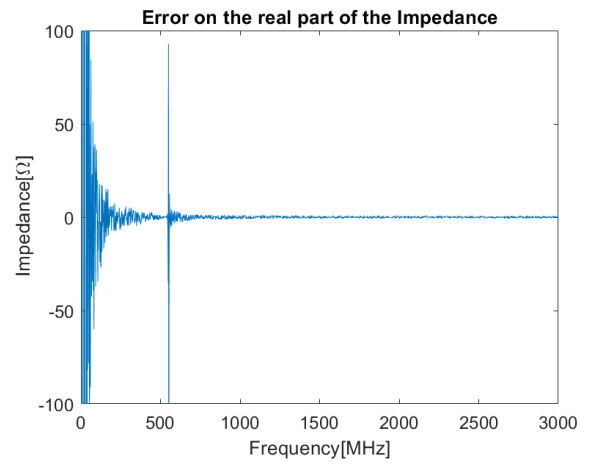


(b)

Figure 4.27



(a)



(b)

Figure 4.28

4.4.5.8 Figures of merit

4.4.5.8.1 Quality factor

The extraction of the quality factor is widely described in section 4.4.5.2.

4.4.5.8.2 Effective coupling coefficient

The extraction of the effective coupling factor is done with equation (3.9). Once the resonance and antiresonance frequencies are found, the only thing remaining is to replace these values in equation (3.9) :

$$k_{eff}^2 = \frac{f_a^2 - f_r^2}{f_a^2}$$

It can also be computed thanks to the lumped elements of the BVD model as shown in equation (4.17).

$$k_{eff}^2 = \frac{C_m}{C_0} \quad (4.17)$$

With C_m and C_0 the motional and static capacitances respectively.

We will favour the first way of extraction (equation 3.9) because it is more direct and does not depend on the extraction of the lumped elements which can contain some errors.

4.4.5.8.3 Resonator FoM

Once the quality factor and effective coupling factor are found, the resonator FoM described in section 3.4.4.3 can be found by replacing the values in equation (3.10).

$$FoM = \frac{k_{eff}^2 Q_r}{1 - k_{eff}^2}$$

4.4.5.8.4 TCF

To compute the TCF, we first have to take measurements at different temperatures. The resonance and antiresonance frequency at each temperature is then extracted. Finally, we used data points for each temperature to extract the relative variation of resonance and antiresonance frequency and performed a first-order linear regression, of which the slope corresponds to the TCF.

Chapter 5

Results

This section presents the results of the analysis of experimental and simulated data from our work. The influence of a number of parameters is assessed by analyzing measurements and models built from the measurements. Then, the performances of the different technologies of interest is evaluated through both measurement and simulation analysis.

5.1 Influence of the photolithography exposition dose

Several parameters are at play when evaluating the performances of a resonator. Fabrication process, substrate, orientation, design geometry and temperature are all factors influencing the performances. In addition, calibration, defaults and operator mistakes can be a source of measurement errors. Therefore, measurement results need to be examined carefully before drawing any conclusions. Hence, it is necessary to assess which parameters have the most significant influence on those results.

In the fabrication process itself, many steps can lead to a change in the final output of the device: baking time and temperature, photoresist adhesion and thickness, photolithography dose and contact, aluminium deposition thickness, lift-off, etc. Even though we tried to keep most of those process parameters constant throughout the fabrication, we are not immune to slight variations, both between wafers and within one wafer itself. Indeed, resist or metal thickness, resist adhesion, lithography and lift-off results can all vary from an area of the wafer to another. Hence, it is very difficult to keep the exact same conditions on the whole wafer. It is also impossible to quantify the impact of these slight differences. Nevertheless, in our result analysis, most conditions are maintained as constant as possible, and only resonators from the same die are compared, thus limiting process variations.

One parameter that is easily quantified is the photolithography exposure dose, as it is a tunable process parameter. The dose has been purposely varied across the wafer to maximize the probability of a satisfactory output. While the impact of the dose is mainly on the fabrication output, this could have an impact on the performances, as lithography impacts the width of the IDT and mirror fingers, and thus also their spacing. In this section, resonators from different exposure doses will be compared, both for bulk LT and POI wafers. The comparison is made using a single type of resonator, in order to isolate the dose as varying parameter. The resonator in question is called "Resonator 1" and has the following specifications : $\lambda = 8 \mu\text{m}$ wavelength, $150 \mu\text{m}$ aperture width, 20 IDT fingers and 10 mirror fingers.

5.1.1 Observations

We can observe the same behavior on both bulk and POI substrates: curves are very close and almost identical, with only a slight shift to higher frequencies and marginally lower admittance values for bigger exposure doses. In the bulk case, there are two resonators from dice with the same exposure (80 mJ/cm^2). However, the curve still differs and one of them is actually closer to the 100 mJ/cm^2 curve. This leads us to believe that the slight variations observed are not a consequence of the

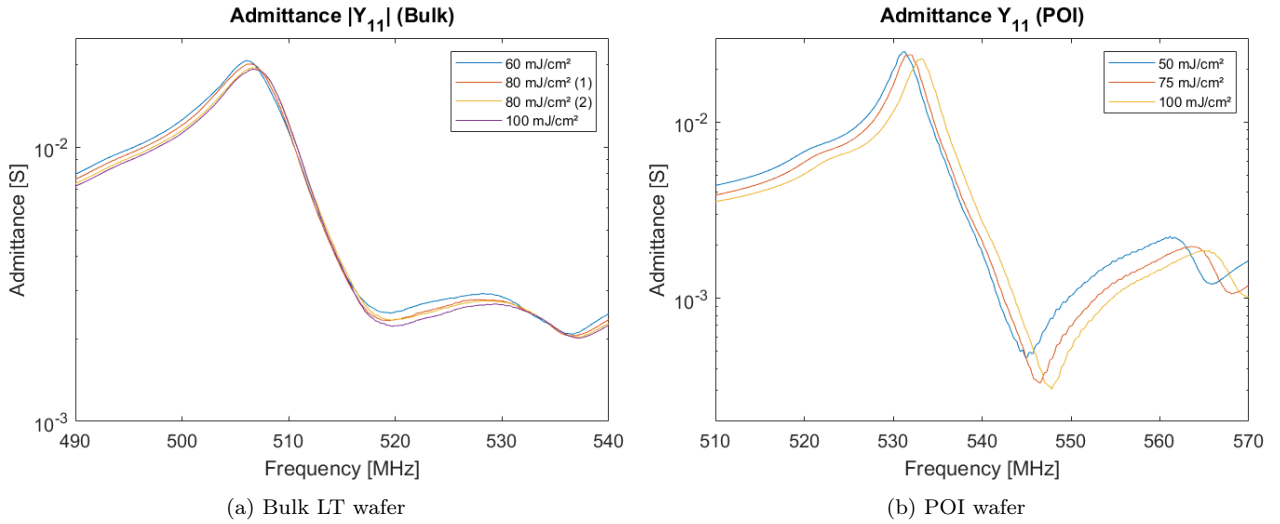


Figure 5.1: Study of the influence of the photolithography exposure dose on the electrical response (illustrated with the admittance) of a resonator.

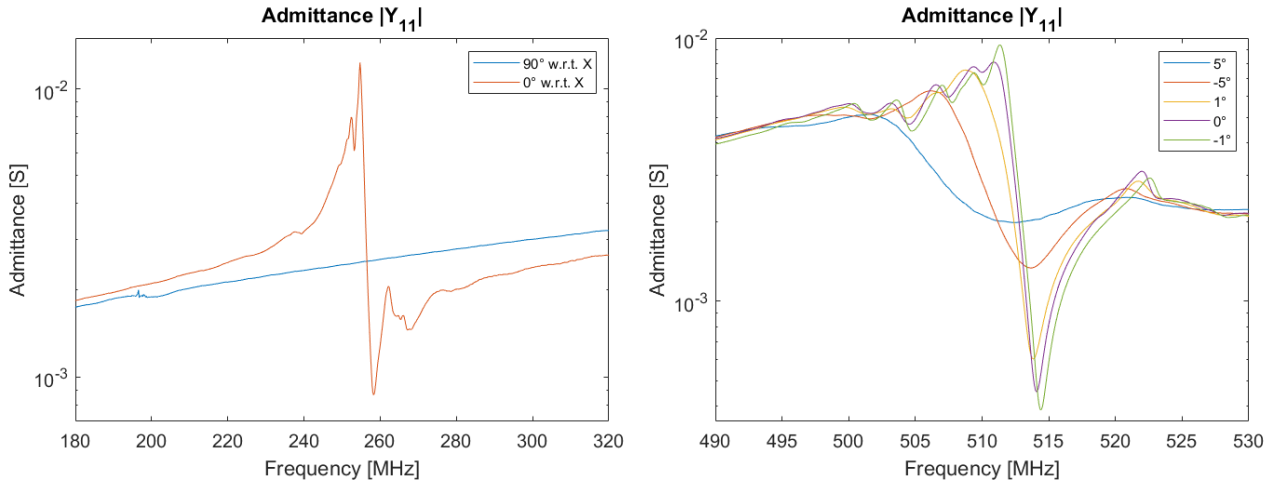
exposure dose difference. As such, we can consider that the exposure dose has little to no impact on the performances, except that they guarantee the proper fabrication of the resonators. Indeed, we have observed that when the dose is too high, there are some cases where the resonators are not even functional, as the finger patterns have not been successfully formed on the wafer.

5.2 Influence of the orientation

Surface acoustic wave propagation is not equal in all directions. The crystal orientation of the wafer has a significant influence on the propagation. Indeed, in the case of 42°Y-X lithium tantalate, propagation is optimal along the X-axis of the crystal. This is actually something we encountered inadvertently when performing our measurements. As we knew that the resonance frequency of a resonator is defined by its geometry (more specifically the pitch of the IDT electrodes), we knew the approximate frequency at which we could expect the resonance to be. However, when performing the measurements, we did not see any resonance at that frequency, and were unsettled by that result. We figured out that this was due to the orientation of the resonators with respect to the crystal X-axis. The resonators had been fabricated with an angle of 90° with respect to the X-axis, hence the poor resonance. We were able to determine this thanks to the layout design of our mask, which included resonators purposely inclined with angles up to 90° . This allowed us to observe that the amplitude of the resonance was highest for those 90° -inclined resonators, which were actually aligned with the X-axis of the crystal. Figure 5.2a shows what could be described as worst and best case of orientation. The two measurements correspond to the exact same resonator (resonator C, presented in appendix A.4, which has a wavelength of $\lambda = 16 \mu\text{m}$) in terms of geometry and fabrication process. Only their inclination changes. We can observe that the resonance is clear in the case of the resonator aligned with the crystal X-axis. For the resonator perpendicular to the X-axis, the resonance at the expected frequency (around 250 MHz ¹ is nonexistent. However, we can observe a much smaller resonance around 200 MHz . This corresponds to a wave with slower velocity, possibly a non-leaky Rayleigh wave.

Wafers of resonators fabricated after we found this were made so that the majority of resonators were aligned with the X-axis. This allows us to use some others resonators with an inclination angle to study the sensitivity of the resonance to a slight variation in that angle. Resonator A (presented in appendix A.4) was used for this study and its possible inclinations are : -5° , -1° , $+1^\circ$ and $+5^\circ$. Resonator A has a wavelength of $\lambda = 8 \mu\text{m}$ and therefore an expected resonance frequency around 500 MHz .

¹The expected resonance frequency is calculated from the wavelength λ and the velocity v of the wave, which is around 4000 m/s for 42°Y-X LT (see section 3.5.1). $f_r = \frac{v}{\lambda}$.



(a) Comparison between resonators parallel and perpendicular to the crystal X-axis (b) Sensitivity of the resonance frequency to the angle variation of the resonator with respect to the crystal X-axis

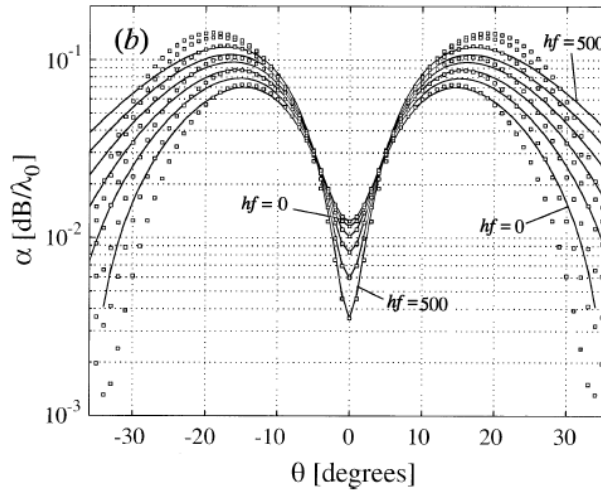


Figure 5.3: Variation of the amplitude attenuation for LSAW propagation in LiTaO_3 as function of the angle with the crystal X-axis

Figure 5.2b shows the admittance of those inclined resonators. We can observe a resonance for all of those resonators, but we can clearly see that the amplitude decreases when the angle with respect to the X-axis increases, with -5° and $+5^\circ$ orientations having the weakest resonance. We can also observe that the best result corresponds to the -1° inclined resonator. Furthermore the $+5^\circ$ case seems worse than the -5° case. This could be explained by a slight misalignment in the fabrication process, which is very plausible. We can conclude that a 1° misorientation is acceptable, but that 5° is too critical of a misorientation to expect correct performances.

The relation between resonator orientation and LSAW amplitude attenuation is verified in the literature (figure 5.3). The graph shows that the attenuation α is minimal for an angle of 0° , in other words a resonator perfectly aligned with the crystal X-axis. Attenuation quickly increases with the inclination angle.

5.3 Geometry Analysis

In this section, we will try to identify the geometry parameters that affect the performances of a resonator. This is achieved by comparing various designs of resonators. The parameters to be studied are the ones described in section 4.2.1: aperture width, number of IDT fingers and number of mirror fingers.

To evaluate the impact of those parameters, we selected a reference resonator, and similar resonators which varied one parameter at a time. Table 5.1 is a summary of the resonators used for

the study and their specifications. Resonator 1 is the reference resonator. Resonators 2, 3 and 4 allowed us to study one isolated parameter at a time, while resonator B varies the number of IDT and mirror fingers simultaneously, and is used to verify our findings.

For each resonator, figures of merit are computed and a model is used to extract equivalent circuit parameters. The method used to determine the values of those parameters is detailed in section 4.4.5. First, the resonance (f_r) and antiresonance (f_a) frequencies are obtained, along with the figures of merit (Q_r , Q_a , k_{eff}^2 , FoM). Then, we use a particular mBVD model to fit the curve. In fact, the first step is to create a BVD model thanks to f_r , f_a and the calculation of C_0 . The BVD model is then plotted, and its data are used to obtain a mBVD model. The effect is that the quality factors computed from the BVD model curve are more reliable than those computed from the measurements data, as they are not prone to noise or errors. The mBVD model lumped elements (C_m , L_m , R_m , R_0 , R_s) are then determined using these newly computed Q factors. The analysis is performed for both resonators built on both bulk lithium tantalate (that we will sometimes simply called "Bulk") and POI wafers in order to confirm the observed results.

Name	Wavelength [μm]	Aperture width [μm]	IDT fingers	Mirror fingers
Resonator 1	8	150	20	10
Resonator 2	8	50	20	10
Resonator 3	8	150	20	100
Resonator 4	8	150	100	10
Resonator B	8	150	100	100

Table 5.1: Resonators used for the geometry analysis study. Key design parameters are listed, with variations from the reference resonator highlighted in bold.

5.3.1 Bulk LT results

The admittance and phase of the admittance curves from which the parameters are extracted are available at Figures 5.4 and 5.5. The parameters extracted from these curves are shown at Tables 5.3 and 5.2. Each resonator can be compared one by one to the reference Resonator 1.

Resonator 2 has a smaller aperture width than Resonator 1. C_0 is thus naturally lower for Resonator 2 as less dielectric material is present between the electrode fingers. Looking at the graphs, the curves of Resonators 1 and 2 are almost identical, except that the admittance of resonator 2 is lower due to the lower C_0 . The difference in C_0 strongly affects the values of motional elements C_m , L_m and R_m . In particular, R_m seems to increase significantly for a reduced aperture width. Besides, R_s is also notably increased. Our hypothesis is that the smaller aperture width lead to a smaller section and thus a higher resistivity in the IDTs. As for figure of merits, they are overall slightly lower for a smaller aperture width.

Resonator 3 has more reflector fingers but the same number of IDT fingers. As a result, C_0 and R_s are very similar compared to Resonator 1. Motional components are not strongly affected, except R_m which is lower. As for the figures of merit, quality factors are higher, which is strongly correlated with the low R_m . Indeed, a high quality factor accounts for small losses. A bigger reflection (due to the higher number of mirror fingers) reduces the losses as the energy is contained within the device. However, the effective coupling factor does not seem to be improved by the number of reflector fingers, with a value lower than for Resonator 1. Indeed, the effective coupling factor signifies that there is a good energy conversion of electrical energy into mechanical energy in the device, which is not enhanced by the reflectors.

Resonator 4 has a higher number of IDT fingers. C_0 therefore naturally increases too, by roughly five times, which is proportional to the number of IDT fingers. The quality factor increases, and R_m decreases strongly compared to Resonator 1. R_s decreases too which can be due to the higher number of fingers in parallel. The resonance and antiresonance are more distant, which yields a higher effective coupling factor. This result is expected as a higher number of IDT fingers converts a bigger part of the energy introduced in the system, resulting in less losses, therefore increasing the quality factor. Furthermore, there are more IDT fingers, hence a higher part of the electrical energy

is converted into mechanical energy, and vice-versa.

It is normal to expect a high effective coupling factor and Q factor from resonator B, which combines a high number of IDT and reflector fingers. The effective coupling factor is indeed quite high but the Q factors are not as high as expected. If we look at the curves, we can see that the curves which come from the measurements for Resonator B (green curves) are really noisy. It can be due to the fact that the structure is bigger, so there can be more defaults or parasitic elements such as parasitic inductances due to the contact pads. It makes the extraction more difficult and the model is thus less accurate than for the other resonators. If we look at the measurements curve, we can still observe that the spacing between resonance and antiresonance is roughly the same as for Resonator 4, which explains that their k_{eff}^2 is close. The slope of the phase is also quite high, the quality factor can thus be quite high even if it is not the case in the extracted model. For those reasons, it is quite hard to have a proper conclusion for Resonator B.

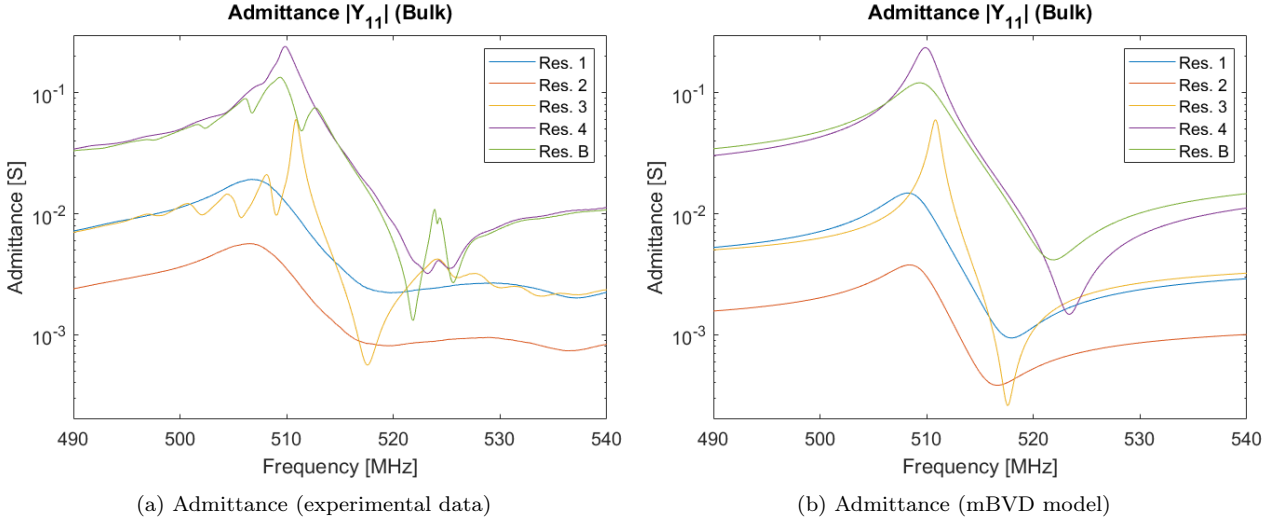


Figure 5.4: Admittance plots for resonators fabricated on bulk lithium tantalate substrate (measurements and mBVD model).

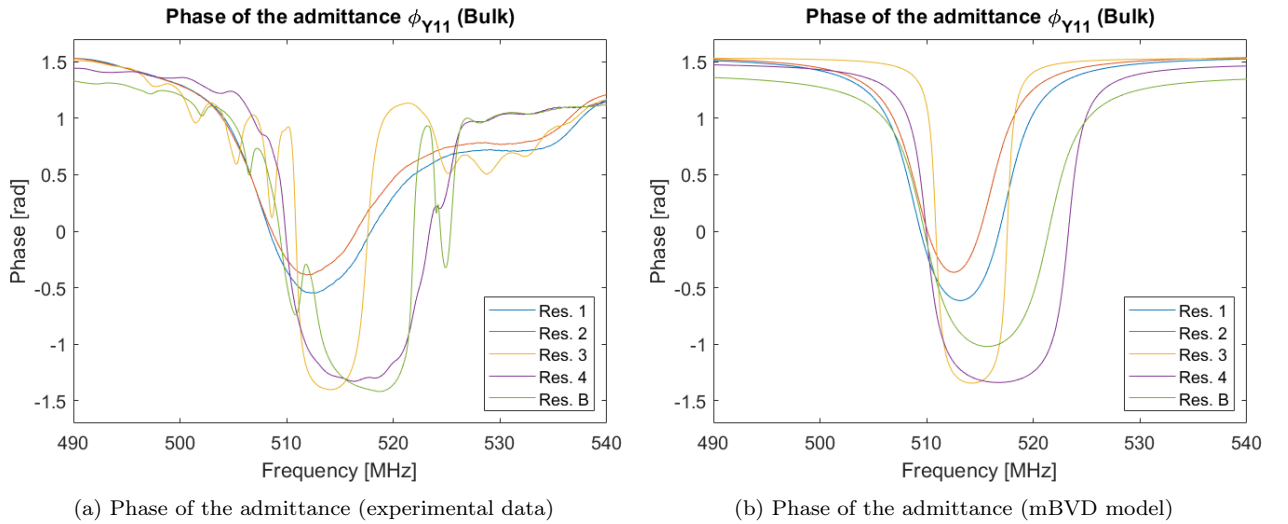


Figure 5.5: Phase of the admittance plots for resonators fabricated on bulk lithium tantalate substrate (measurements and mBVD model).

Bulk	f_r [MHz]	f_a [MHz]	Q_r [/]	Q_a [/]	Q_r^M [/]	Q_a^M [/]	k_{eff}^2 [/]	FoM [/]	FoM^M [/]
Res. 1	508.34	517.91	76.4	40.2	109.4	111.5	3.66%	2.90	4.15
Res. 2	508.59	516.50	60.7	46.1	106.1	107.8	3.04%	1.90	3.33
Res. 3	510.84	517.59	718.8	363.4	570.5	578.1	2.59%	19.12	15.18
Res. 4	509.88	523.38	268.8	156.1	237.7	244.0	5.09%	14.43	12.75
Res. B	509.31	521.88	186.3	634.2	111.9	114.1	4.76%	9.30	5.59

Table 5.2: Figures of merit of five resonators with different geometric parameters, built on a bulk lithium tantalate wafer. All five resonators come from the same die with an exposure of 100 mJ/cm². Subscript "M" stands for model. Q_r , Q_a and FoM are directly extracted from the measurements while Q_r^M , Q_a^M and FoM^M are extracted from the mBVD model which is built with the the lumped elements of Table 5.3.

Bulk	C_0 [fF]	C_m [fF]	L_m [μH]	R_m [Ω]	R_0 [Ω]	R_s [Ω]
Resonator 1	1169.9	39.9	2.46	67.74	1.50	4.01
Resonator 2	376.0	10.0	9.74	283.09	2.06	10.39
Resonator 3	1229.7	32.6	2.98	12.04	4.29	4.73
Resonator 4	5848.0	310.1	0.31	2.03	1.99	2.20
Resonator B	7075.8	331.8	0.29	4.39	3.67	4.01

Table 5.3: Lumped elements of the mBVD model equivalent circuit for 5 resonators with different geometries built on a bulk lithium tantalate wafer. All five resonators come from the same die with an exposure of 100 mJ/cm².

5.3.2 POI results

Equivalent circuit parameters and figures of merit are available at Tables 5.5 and 5.4 respectively. Admittance curves from measurements and the mBVD model are available in Figure 5.6 while phase curves from measurements and mBVD model are available in Figure 5.7.

Once again, there are no big differences for the figures of merit between Resonator 1 and Resonator 2, even as C_0 is more or less three times lower for Resonator 2.

Resonator 3, with ten times more reflector fingers presents much higher quality factors than Resonator 1. As explained for Bulk resonators, reflectors reduce the losses and therefore increase the quality factor. Nevertheless this does not increase the coupling coefficient factor which is even lower than for Resonator 1. Indeed, reflectors reduce the losses but do not increase the conversion between electrical and mechanical energy.

Resonator 4 has a higher number of IDT fingers and a associated higher C_0 . We can also observe a decreased series resistance R_s , which might also be due to the high number of fingers. The quality factor and effective coupling factor are higher for Resonator 4 compared to Resonator 1. As explained for Bulk resonators, increasing the number of IDT fingers increases the conversion of electrical to mechanical energy and also reduces the losses. Both figures of merit (k_{eff}^2 and Q-factors) are thus increasing.

Resonator B is once more quite noisy, which may be due to parasitical elements. The result is that the mBVD model is hard to extract and can be a bit biased. Still, the effective coupling factor is the highest between all the resonators. Quality factors computed from the model are in the same order of magnitude as Resonator 1. But quality factors directly extracted from measurements are much higher than for Resonator 1 and 2. It is thus hard to have proper conclusion concerning quality factors for Resonator B.

5.3.3 Conclusion of the geometry study

From both analyses some conclusions arise. First, the proportional relation between C_0 and the number of IDT fingers is clear. C_0 also seems to increase with an increasing aperture width. The, R_s also seems highly affected by the number of fingers. An increased number of fingers decrease R_s , but a overall big size of the resonator can compensate this effect. Besides, a reduced aperture width seems to have an increasing effect on both R_s and R_m . In terms of figures of merit, there seems to be a relationship between the number of reflectors and the quality factors. Indeed the purpose of

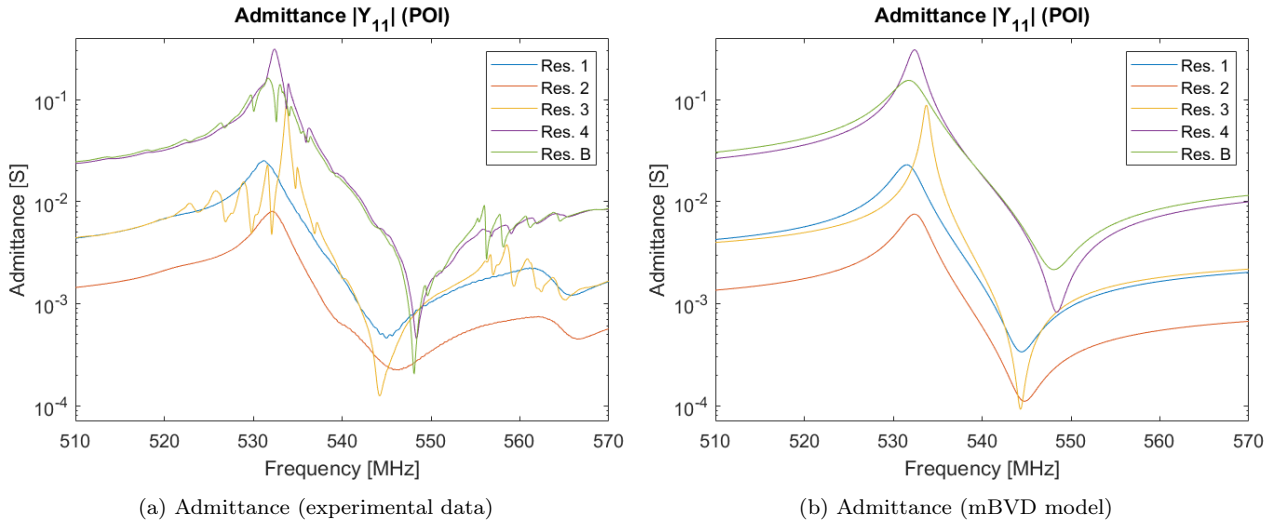


Figure 5.6: Admittance (measurements and mBVD model)

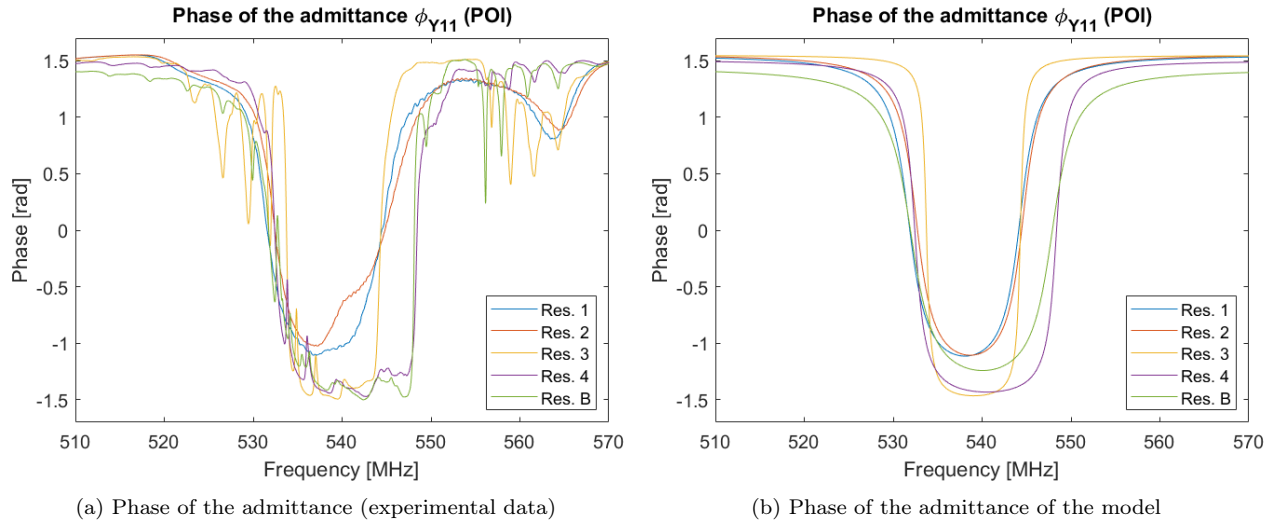


Figure 5.7: Phase of the admittance (measurements and BVD model)

the reflectors is to reflect the waves which go out of the device back to the device with constructive interferences. We therefore expect a higher quality factor when the number of reflector fingers is increased, and this is exactly what we observe. However, it does not impact the effective coupling factor. Indeed the number of reflectors does not affect the conversion of electrical to mechanical energy. The coupling factor even decreases in both bulk and POI cases. There is also a relationship between the number of IDT fingers, the quality factor and the effective coupling factor. As there are more IDT fingers, there is more energy which is converted, the energy losses are thus reduced and the energy conversion is also increased. Both figures of merit presented here are thus increased.

POI	f_r [MHz]	f_a [MHz]	Q_r [/]	Q_a [/]	$Q_{r,m}$ [/]	$Q_{a,m}$ [/]	k_{eff}^2 [/]	FoM [/]	FoM_m [/]
Res. 1	531.56	544.46	134.7	74.6	170.1	174.2	4.68%	6.62	8.36
Res. 2	532.43	544.80	208.7	65.3	178.2	182.3	4.49%	9.81	8.38
Res. 3	533.74	544.35	1281.6	548.3	773.0	788.4	3.86%	51.47	31.05
Res. 4	532.39	548.44	466.0	782.0	317.3	326.9	5.77%	28.52	19.42
Res. B	531.71	548.10	277.5	858.4	137.1	141.3	5.89%	17.37	8.58

Table 5.4: Figures of merit of five resonators with different geometric parameters, built on a POI wafer. All five resonators come from the same die with an exposure of 50 mJ/cm². Subscript "M" stands for model. Q_r , Q_a and FoM are directly extracted from the measurements while Q_r^M , Q_a^M and FoM^M are extracted from the mBVD model which is built with the the lumped elements of Table 5.5.

POI	C_0 [fF]	C_m [fF]	L_m [pH]	R_m [Ω]	R_0 [Ω]	R_s [Ω]
Resonator 1	830.5	39.7	2.26	39.66	2.60	4.65
Resonator 2	272.5	12.5	7.17	125.01	3.64	9.61
Resonator 3	849.3	34.0	2.62	7.23	3.69	4.12
Resonator 4	4757.4	289.1	0.31	1.13	1.95	2.13
Resonator B	5480.6	334.1	0.27	2.68	3.48	3.86

Table 5.5: Lumped elements of the mBVD model equivalent circuit for 5 resonators with different geometries built on a POI wafer. All five resonators come from the same die with an exposure of 50 mJ/cm².

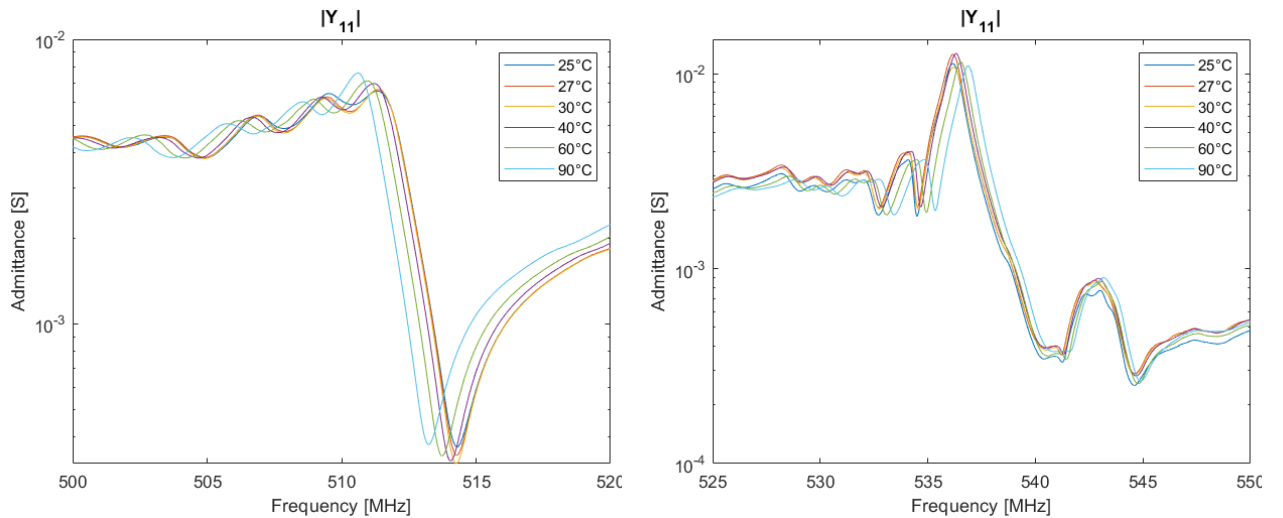
5.4 Influence of the temperature

We assessed whether the temperature had an influence on the performance of the resonators. This was achieved thanks to a ThermoChuck which allows to control the temperature. We started at 25°C, which is the standard temperature, and the one used for many physical properties in our simulation (Comsol).

Another important parameter which can influence the performance of the resonators is the temperature. Hence, we evaluated the sensitivity of the performance to the temperature. Stability with regard to temperature is supposed to be one of the main qualities of the POI wafers [27].

In this section, we will therefore extract the TCF for both bulk and POI LiTaO₃ wafers, then compare the results to the literature.

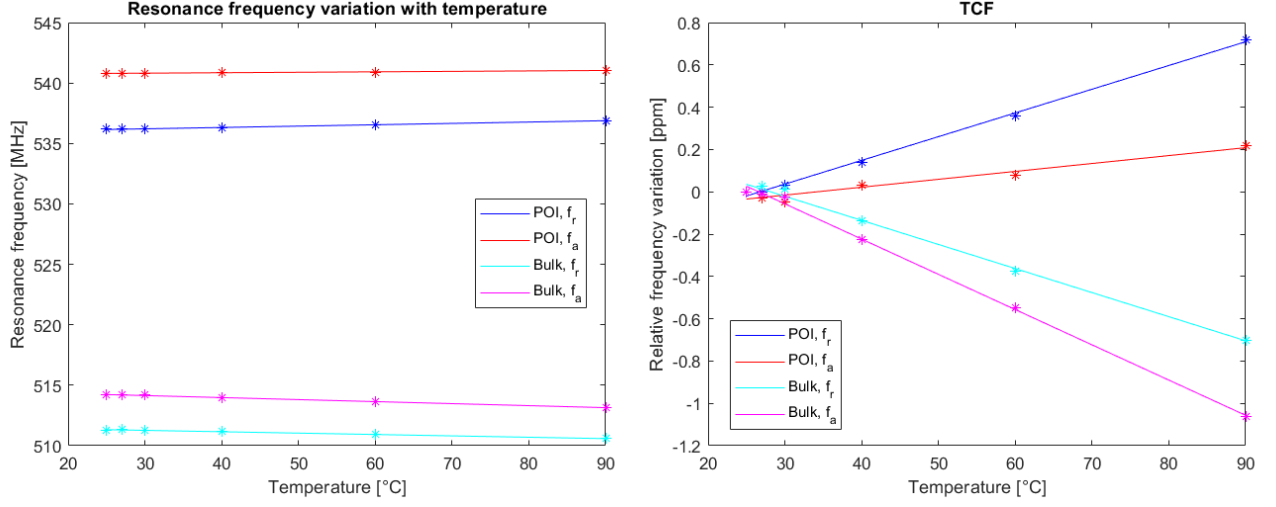
In order to achieve this, we used a probe station chuck that allows for temperature control, or ThermoChuck. It allows for precise temperature control over a wide range. As cooling takes much longer than heating, we increased the temperature gradually in order to perform our measurement efficiently. Temperatures used were 25, 27, 30, 40, 60 and 90°C.



(a) Variation of admittance with temperature increase - Bulk (b) Variation of admittance with temperature increase - POI

Figure 5.8: Variation of admittance with temperature increase

We can observe on figure 5.8 that temperature does indeed have an impact on the resonance frequency of the resonators. Interestingly, this influence is different on both materials. On the bulk LiTaO_3 substrate (figure 5.8a), the resonance seems to shift towards lower frequencies at higher temperatures, while on the POI (figure 5.8b) it seems to shift towards higher frequencies.



(a) Resonance and antiresonance frequency evolution with temperature

(b) Temperature coefficient of frequency evolution with temperature

Figure 5.9: Combined experimental results for bulk and POI

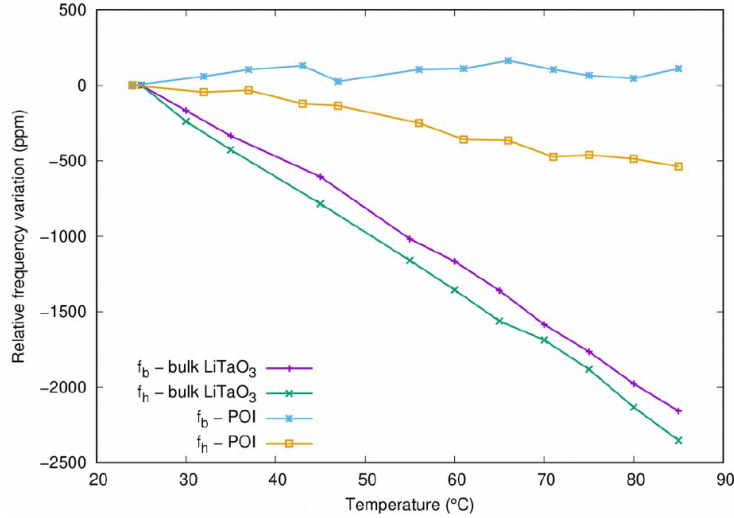


Figure 5.10: Comparison of the TCF for bulk and POI LiTaO_3 resonators [27]

While observing the admittance plot already gives an idea of the effect of the temperature on the resonators, it is necessary to introduce a more quantified figure of merit for this characteristic. The temperature coefficient of frequency (TCF) is used for this purpose, and is defined as the normalized variation of frequency with temperature (5.1) and is usually described in units [ppm/K].

$$TCF = \frac{1}{f} \frac{df}{dT} \quad (5.1)$$

Figure 5.9a shows the evolution of resonance (f_r) and antiresonance (f_a) frequencies with temperature increase, for both bulk and POI substrates. This variation is then transformed into a relative variation by dividing it by the resonance/antiresonance at 25°C. The slope of this relative variation with the temperature gives the TCF, which is illustrated on figure 5.9b. Numerical results are gathered in table 5.6.

Results	TCF (f_r) [ppm/K]	TCF (f_a) [ppm/K]
Bulk	-22.2586	-32.4069
POI	20.9146	6.9075

Table 5.6: Experimental TCF results

Results	TCF (f_r) [ppm/K]	TCF (f_a) [ppm/K]
Bulk	-29.8	-36.6
POI	4.9	-8.6

Table 5.7: Literature TCF results

Now, it is useful to compare those results with others found in the literature. We used results coming from a paper partly written by members of SOITEC themselves, which guarantees the closest working condition to ours, as the same substrates (both bulk and POI) of LiTaO_3 are used [27]. Note that in that work, f_b (from French "bas", for lower filter edge) and f_h (from French "haut", for higher filter edge) are used to designate f_r and f_a , respectively. Table 5.7 gathers results from the aforementioned paper. We can observe that TCF values for the POI substrate are higher and (close to) positive, while they are negative for the bulk substrate, similarly to our results. While POI values differ from ours, Bulk values are very close to what we have obtained, thus validating our measurements.

5.4.1 Observations

We can now claim that although the temperature has a tangible impact on the resonators, this impact is negligible when the temperature difference is of the order of 1°C . Indeed, in absolute value, the TCF is never much higher than 30 ppm/K, which means that a variation of 1°C in temperature can induce, for resonance frequencies of hundreds of MHz (10^8 Hz), a variation of 100 Hz in the resonance or antiresonance frequency. Hence we can consider that all of our measurements are done in the same conditions of temperature, as the laboratory room temperature is always close to 25°C .

5.5 Technology comparison

The three technology options can now be compared using real life measurements and simulation results.

5.5.1 Comparison using experimental data

As explained before, only bulk lithium tantalate (LT) and POI technologies could be measured as we had no AlN wafer at our disposal. In this section, bulk LT and POI substrates are compared. In order to achieve that, the parameter values of the model are extracted in both cases, and their figures of merit are computed. Furthermore, plots of the admittance and its phase are presented to provide a graphical understanding.

5.5.1.1 Method

As was the case for previous studies, a particular method of modelling is used in this study. The procedure is as follows. The starting point is a BVD model parameter extraction, as those parameters only depend on the resonance and antiresonance frequencies, and the determination of the static capacitance C_0 . Simultaneously, a mBVD model parameter extraction is performed for comparison purposes. The mBVD parameters further depend on the Q factor at resonance and antiresonance. The Q factors are very sensitive to data perturbations such as noise. As raw measurement data often shows a lot of these perturbations, the calculation of the Q factor is error-prone. As such, the mBVD parameter extraction can be inaccurate. One way to adress this issue is by performing the mBVD parameter extraction on a new set of data, obtained by using the parameters of the

BVD model extraction. This way, the mBVD extraction is performed on a model which is closer to theoretical curves and therefore yields more consistent results. This second mBVD extraction produces the model that fits the experimental data the best.

5.5.1.2 Comparison using measurements

In this section, only the measurements are used to compare bulk and POI technologies. Figures of merit can be calculated based on the measurement data, using the methods described in section 4. Three resonators (Resonators 1, 3 and 4) are used for this study.

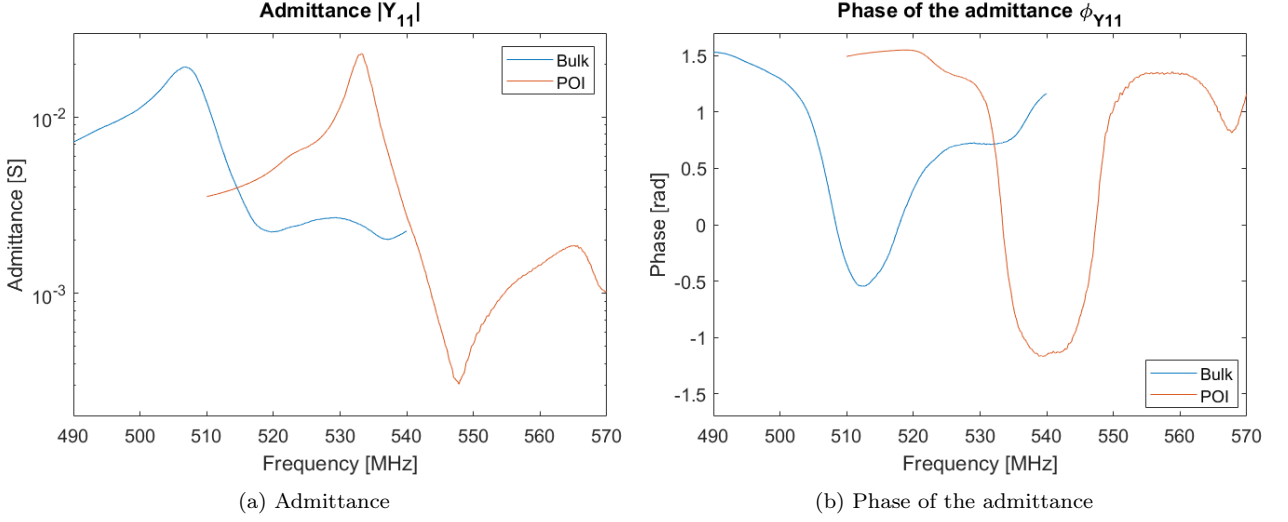


Figure 5.11: Resonator 1: comparison of bulk and POI substrates using measurements.

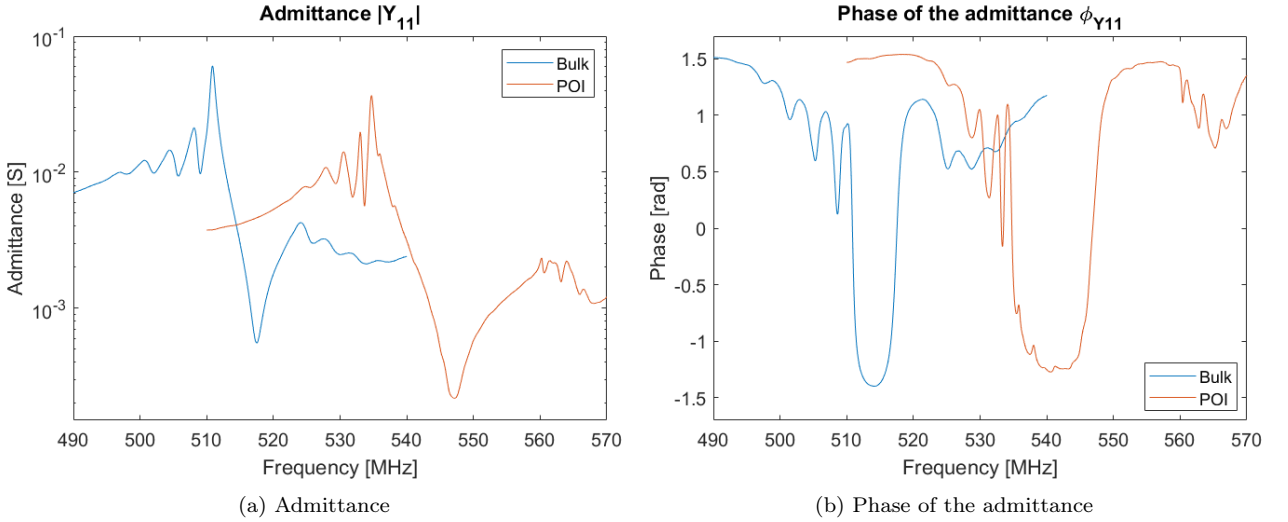


Figure 5.12: Resonator 3: comparison of bulk and POI substrates using measurements.

5.5.1.2.1 Observations

At this stage, a few observations can be made, which we will try to confirm with the models. first, we can observe higher resonance and antiresonance frequencies for the resonators fabricated on POI wafers. While the difference is relatively small, this means a higher velocity for the waves travelling in the POI substrate, which is favorable.

Besides, the figures of merit of the POI case are generally higher than for the bulk case, with the notable exception of the Q factors of Resonator 3. Higher Q factors are expressed visually through steeper slopes of the phase plot. A higher effective coupling factor can be detected via a wider range

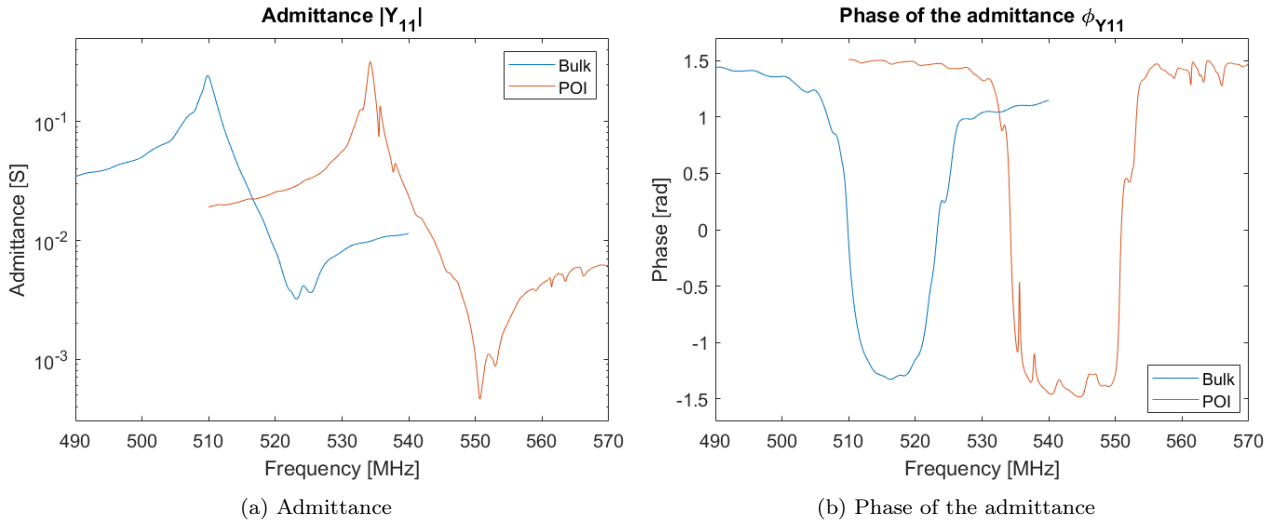


Figure 5.13: Resonator 4: comparison of bulk and POI substrates using measurements.

Resonator	f_r [MHz]	f_a [MHz]	Q_r [/]	Q_a [/]	k_{eff}^2 [/]	FoM [/]
Resonator 1, Bulk	508.3	517.9	76.4	43.5	3.65%	2.89
Resonator 1, POI	533.4	547.3	185.4	128.6	5.03%	9.83
Resonator 3, Bulk	510.8	517.5	718.9	367.9	2.57%	18.94
Resonator 3, POI	534.8	546.9	722.3	223.7	4.38%	33.09
Resonator 4, Bulk	509.9	523.3	268.8	169.3	5.06%	14.32
Resonator 4, POI	534.2	550.8	537.9	482.9	5.94%	33.97

Table 5.8: Measurements comparison

separating the resonance and antiresonance frequencies. Both these characteristics can be observed on the graphs in Figures 5.11, 5.12, 5.13. This is also in line with the claims of the POI manufacturer, Soitec.

5.5.1.3 Comparison using models

Having observed the effect of the choice of substrate on the measurement data, we will try to validate it by producing models for each of those resonators. The modelling process is described earlier, and uses a combination of BVD and mBVD models. A parameter extraction is then performed using the model.

Resonator	f_r [MHz]	f_a [MHz]	Q_r [/]	Q_a [/]	k_{eff}^2 [/]	FoM [/]
Resonator 1, Bulk	508.8	517.4	109.4	111.5	3.28%	3.71
Resonator 1, POI	533.5	547.2	184.4	189.2	4.94%	9.58
Resonator 3, Bulk	510.8	517.5	568.4	575.8	2.56%	14.91
Resonator 3, POI	534.8	546.8	319.1	326.3	4.34%	14.48
Resonator 4, Bulk	509.9	523.2	237.3	243.6	5.00%	12.49
Resonator 4, POI	534.2	550.8	448.9	462.8	5.93%	28.28

Table 5.9: Technology comparison : resonance and antiresonance frequencies and figures of merit extracted from the model.

5.5.1.4 Observations

Most observations made about the measurement analysis hold true when using the model as comparison basis. Resonance and antiresonance frequencies, which are used to build the model, have almost

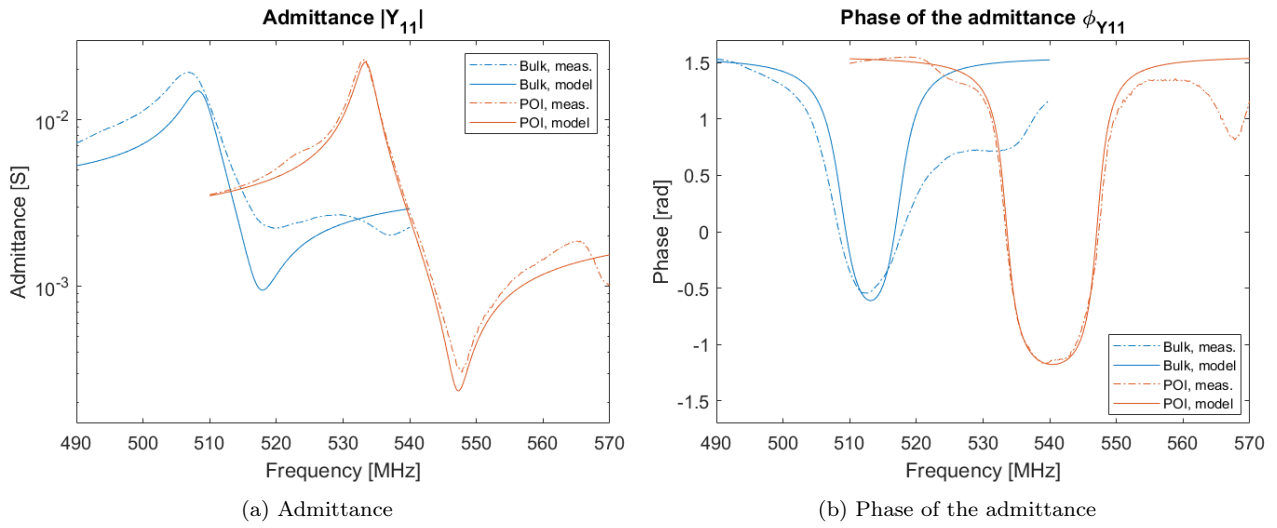


Figure 5.14: Resonator 1: comparison of bulk and POI substrates using the mBVD model. Measurement data are represented with dotted lines.

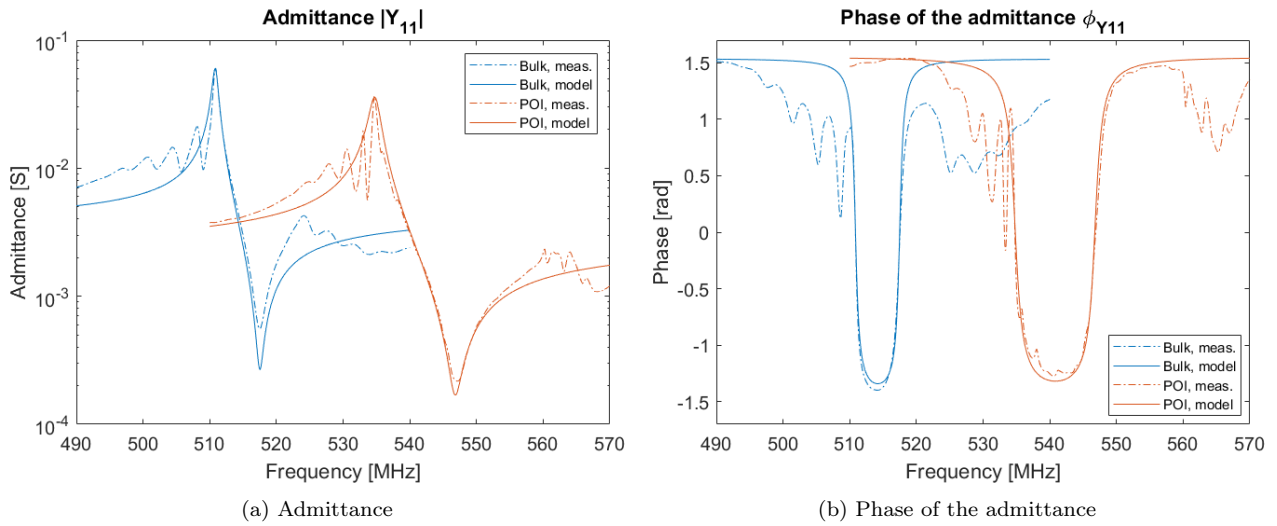


Figure 5.15: Resonator 3: comparison of bulk and POI substrates using the mBVD model. Measurement data are represented with dotted lines.

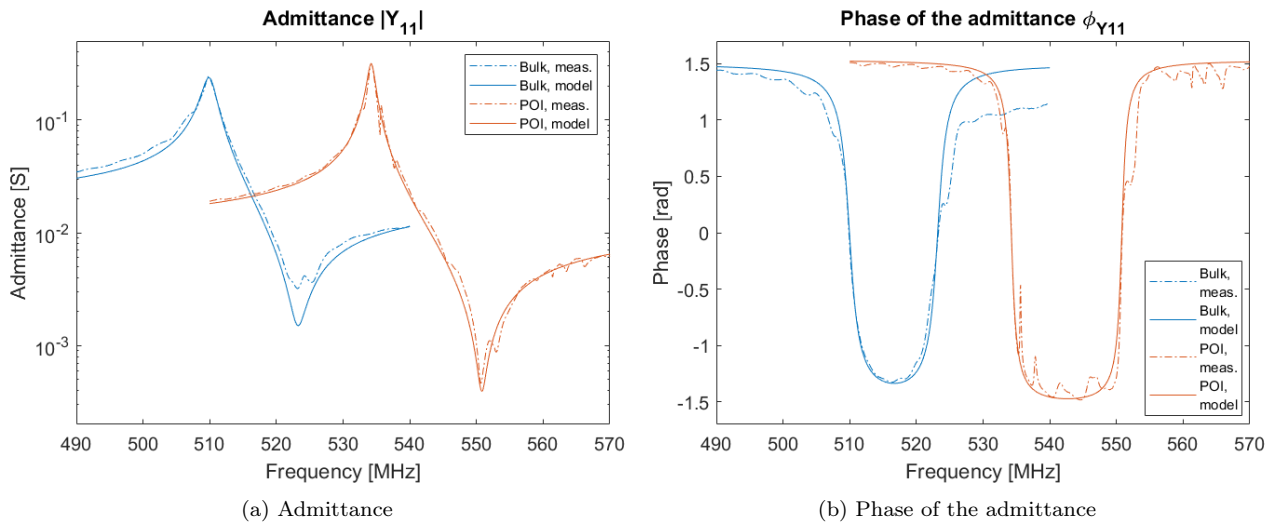


Figure 5.16: Resonator 4: comparison of bulk and POI substrates using the mBVD model. Measurement data are represented with dotted lines.

Resonator	C_0 [fF]	C_m [fF]	L_m [μH]	R_m [Ω]	R_0 [Ω]	R_s [Ω]
Resonator 1, Bulk	1173.4	39.83	2.457	67.80	1.50	4.00
Resonator 1, POI	679.4	35.31	2.521	41.85	1.68	3.97
Resonator 3, Bulk	1245.7	32.67	2.971	12.19	4.16	4.59
Resonator 3, POI	731.4	33.19	2.668	23.60	3.27	4.50
Resonator 4, Bulk	5898.0	310.49	0.314	2.05	1.97	2.18
Resonator 4, POI	3311.7	208.68	0.425	1.27	1.72	1.91

Table 5.10: Technology Comparison : equivalent circuit parameters extracted from the model.

not changed and there remains a slight shift in frequency between bulk and POI resonators. The same can be said of the effective coupling factors, which have changed slightly, but remain higher for the POI case. As for the quality factors, they are greatly impacted by the switch from measurement to model, as the model curves are much more ideal than the measurements which can be noisy. Q factor computation from models is much more consistent than the equivalent computation from the experimental data. We can observe closer values of resonance and antiresonance Q factors, while in the case of measurements, Q factor values could be very high or very low depending on the noise on the data. Still, we generally observe higher Q factors for the POI substrate, despite Resonator 3 still displaying lower Q factors than for the bulk substrate.

As for the quality factors, the figure of merit for resonator (FoM) are really higher for POI than for bulk LT (except for resonator 3 where both have the same order of magnitude). POI substrates seem thus to be better candidate for SAW resonator than bulk LT.

Further observations can be made based on the extraction of the equivalent circuit parameters from the mBVD model (Table 5.10). First, C_0 , the static capacitance of the IDT, is higher for the bulk case. This can be explained by the fact that more dielectric material (in this case, the piezoelectric LT, which is the surface layer) is present in the bulk case. Besides, it is worth noting that the series resistance R_s remains almost constant between bulk and POI substrates. R_s corresponds to the resistance of the electrical components external to the resonator itself, such as the bus bars and contact pads; parts which are theoretically identical as they are made from aluminium in both bulk and POI cases. Hence, this result is coherent.

Having validated our observations by comparing measurement data and models derived from this data, we will now compare it with simulation results.

5.5.2 Technology analysis - Simulation

In this section, we will use COMSOL simulations in order to compare the three technologies. Simulation limitations mean that the reference resonator used for this purpose is a simplified version of the ones we have in real-life, with only a single pair of IDT fingers.

Simulation for resonance mode of POI, bulk LT and AlN are available at Figure 5.17, 5.18 and 5.19 respectively. Some things can already be noticed such as the fact that the SAW resonance mode correspond to the resonance on the admittance plot. Furthermore the guided waves are rather clear on Figure 5.17 where the energy is concentrate in a thin layer. Then the frequency studies with phase and admittance are shown at figure ??, ?? and 5.19 for POI, bulk LT and AlN respectively. The admittance and phase of the BVD model extracted from the simulations are also shown on these graphs. BVD model is prefer to mBVD model in this case because R_s makes no sense as the resistance of the IDTs is not introduced in COMSOL.

There are some limitations to the simulations. First of all when we look at the Figure ??, there is some kind of noise which is not there on the measurements. It can be due to interferences with other resonance mode, or due to a too big mesh (unfortunately the simulations were too heavy for our computers with a finer mesh). In all the case, it does not seem to be "normal" and it is a limitation of the simulation.

About the POI, we can emit some doubts about its the quality factor. It is higher than the one of

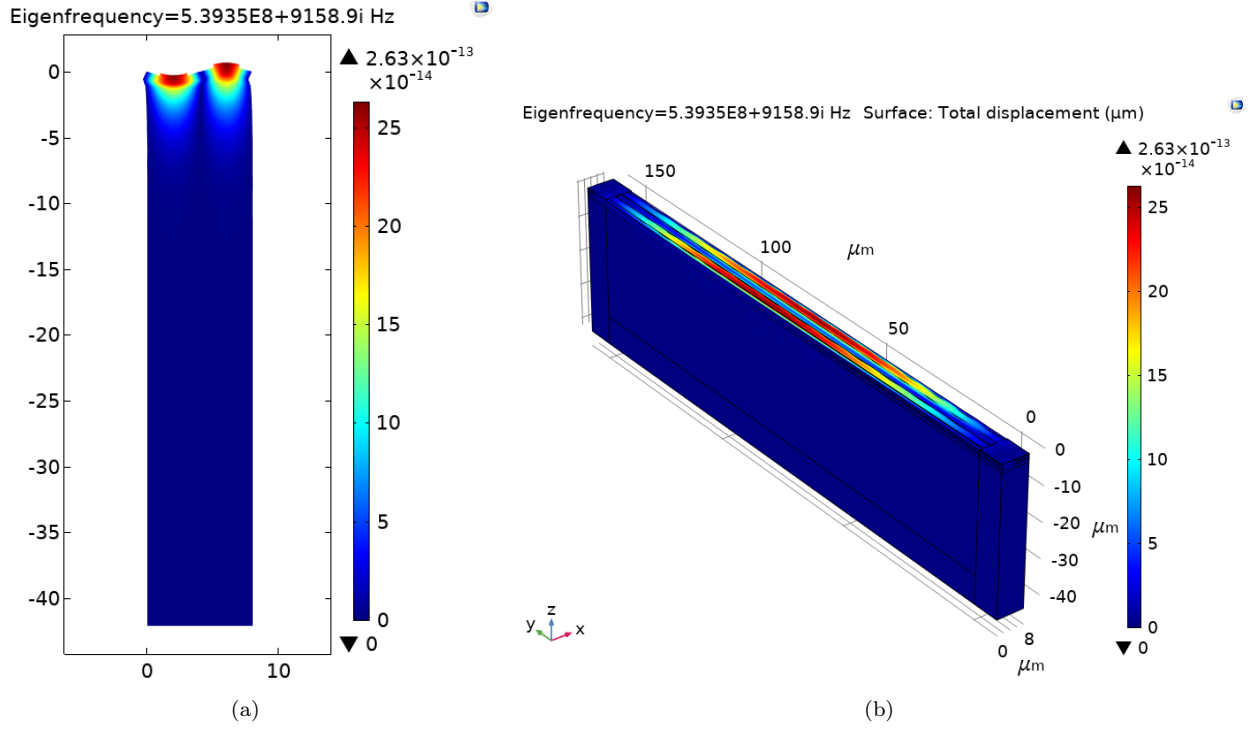


Figure 5.17: COMSOL simulation of the resonance mode of resonator on POI substrate

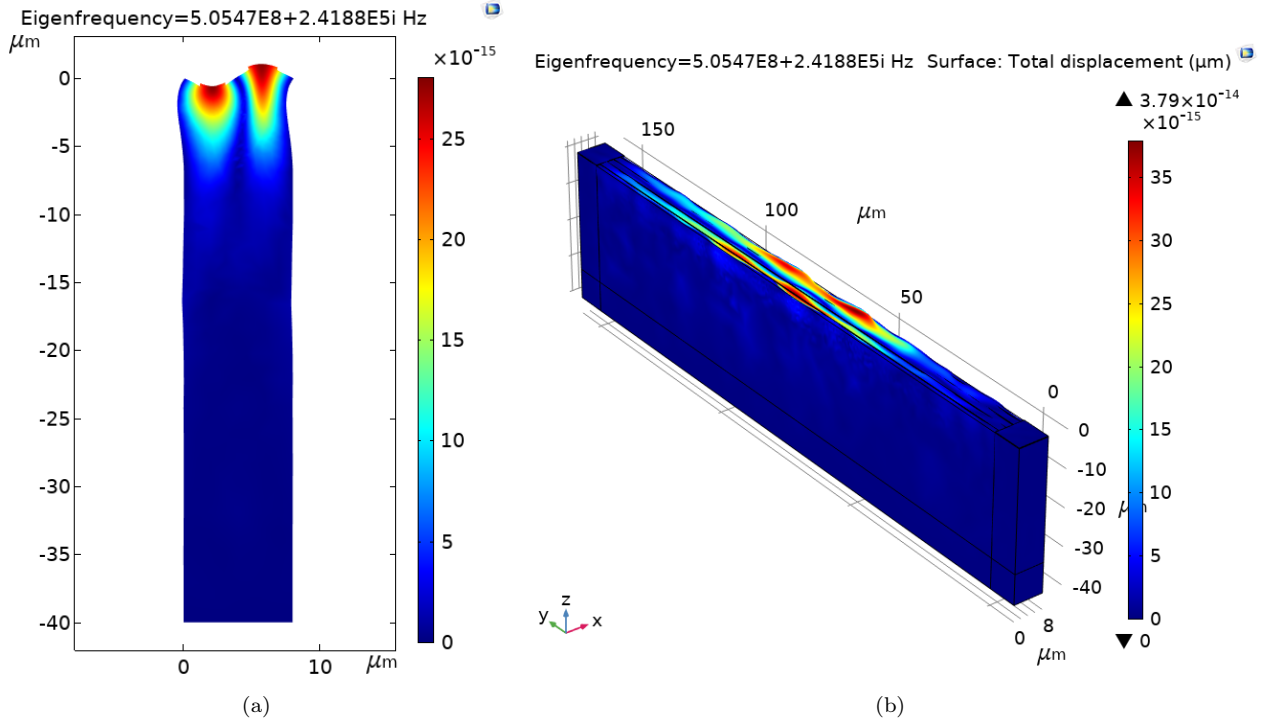


Figure 5.18: COMSOL simulation of the resonance mode of resonator on bulk LT substrate

the bulk LT which is also what we observe with measurements. But it is so high compare to the other that is seems unreal. It can be due to the fact that only the dielectric losses are introduced in the COMSOL model and that the dielectric layer is much smaller than in the other models. It is also a limitation of the simulations.

The figure of merit for resonator is naturally much higher for the POI due to the high quality factor. Then the poor effective coupling factor of the AlN induces a worse figure of merit than $LiTaO_3$ which seems thus more suitable for SAW than AlN.

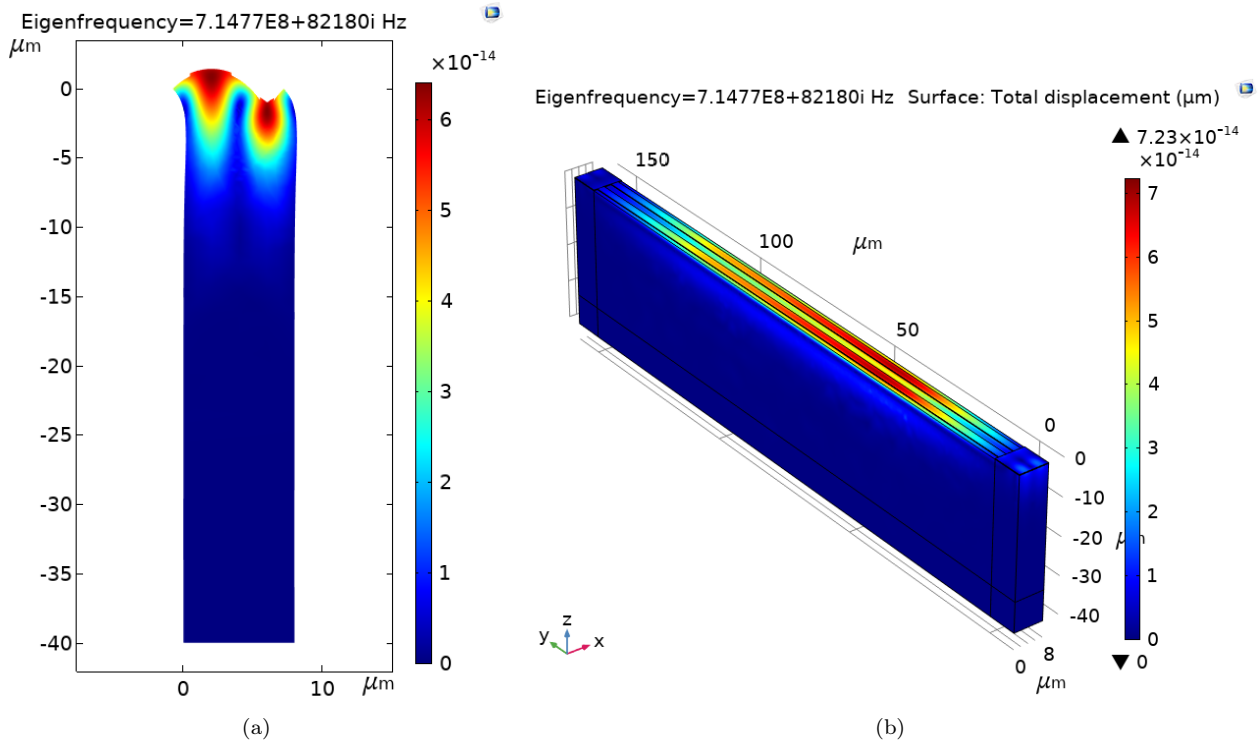


Figure 5.19: COMSOL simulation of the resonance mode of resonator on AlN substrate

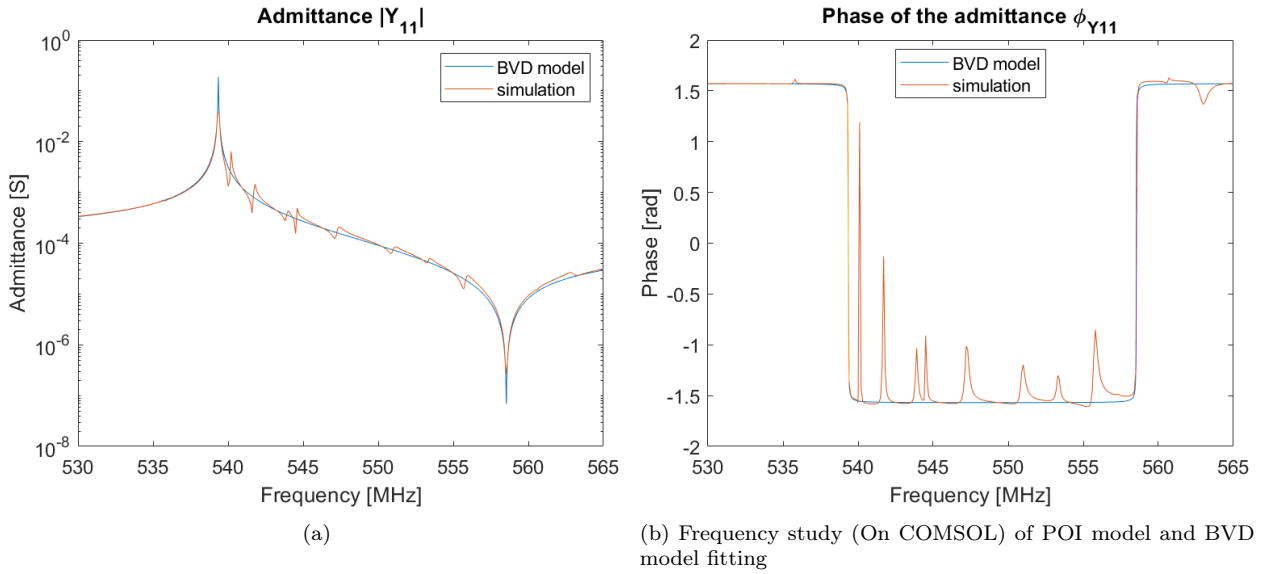


Figure 5.20

The observations which can be done based on simulations confirmed the observations done based on measurements and are in accordance with the literature.

The first point about the lumped element is that C_0 is much higher for bulk LT, it is naturally smaller for POI because the layer of dielectric is smaller, at it is even smaller for AlN. It is due to the lower relative permittivity of AlN compare to LiTaO_3 . The value of other lumped element depend on C_0 , resonance, antiresonance and quality factor. It is difficult to give conclusion just based on it.

The resonance and antiresonance frequencies are really close to the one expected. The speed of Leaky wave in LT and Rayleigh wave in AlN are more or less 4200 m/s and 5760 m/s respectively. If we divide it by the wavelength (8 μm) we find 525 MHz for LT and 720 MHz for AlN. Speed of AlN is much faster than in LT, it is confirmed by simulations, it will allows to reach much higher frequencies with the same accuracy of lithography and thus extend the range of frequency of SAW.

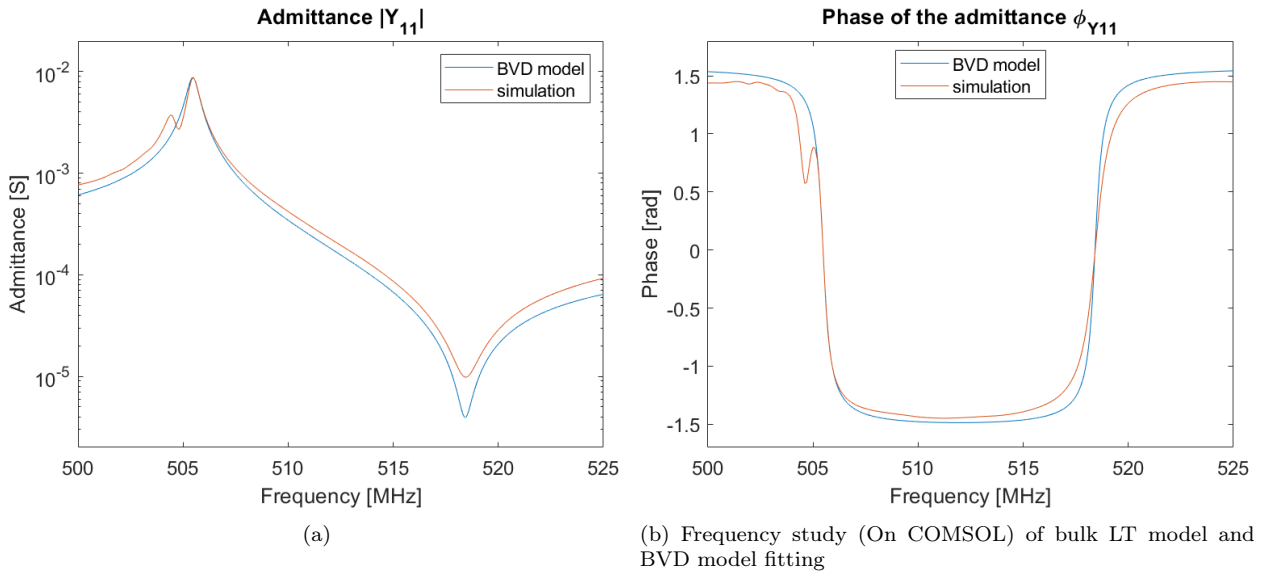


Figure 5.21

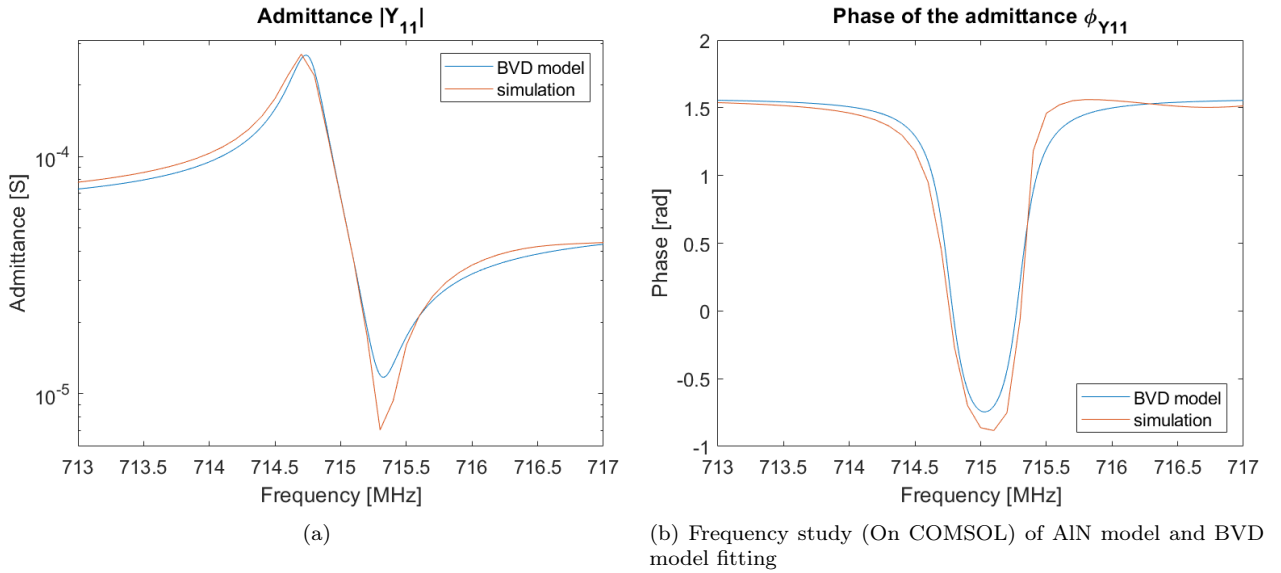


Figure 5.22

Then the speed is also higher in POI than in bulk LT which was the result expected by Soitec, it could also allow to push the upper limit of frequency for SAW a bit higher.

The quality factors, either for measurements directly or for BVD model extracted from it, go in the same way. The quality factor of POI is much higher than the others, it is the wish of Soitec but as explained in the beginning of the section we will not conclude anything from that. The rest goes completely in the way of literature. Higher quality factors can be reach with AlN.

Last but not least, the effective electromechanical coupling factor is also as expected. The coupling factor of AlN is its main drawback, it is smaller than 1% and unfortunately this is what is seen in literature. The coupling factor of POI is higher than the one of bulk LT, it is what we saw on the measurement, and it is the expected result from Soitec study even if the coupling factor of POI resonator can reach 9% is literature [24].

We can also compare the value and order of magnitude of lumped element and figure of merit from simulation on one side and measurements on the other side.

C_0 is higher for measurements, but remember that simulation is done for one pair of IDT. If we multiply the value of C_0 obtain with simulation by the number of pair of IDT in Resonator 1

	L_m [μ H]	C_0 [fF]	C_m [fF]	R_m [Ω]
POI	37.33	32.22	2.3324	5.372
Bulk LT	33.47	57.07	2.9618	114.196
AlN	2630.23	12.47	0.0189	3908.301

Table 5.11: BVD lumped element extracted from simulation over COMSOL models

	f_r [MHz]	f_a [MHz]	Q_r [/]	Q_a [/]	$Q_{r,BVD}$ [/]	$Q_{a,BVD}$ [/]	k_{eff}^2 [/]	FoM [/]	FoM_{BVD} [/]
POI	539.35	558.53	22491.43	24866.57	23490.91	24326.28	6.750%	1628.09	1700.44
Bulk LT	505.47	518.42	990.75	504.72	930.14	953.97	4.934%	51.42	48.27
AlN	714.76	715.3	2622.50	5291.83	2714.49	2716.56	0.151%	3.96	4.10

Table 5.12: Figure of merit extracted from simulation and from BVD model with lumped element at Table 5.11

(20) for example, we obtain 644.4 fF for POI and 1141.4 fF for bulk, which is really close to the measurements. Resonance and antiresonance frequencies are also very similar between simulation and measurements for both POI and bulk LT. It results that the ratio C_m/C_0 should be almost equal for measurements and simulation and it is the case. The product $L_m \times C_m$ determines resonance. Because resonance is almost the same between measure and simulation, the product must be in the same order of magnitude, which is the case too.

The effective coupling factor is a bit higher for simulation model, which is an ideal model, but in the same order of magnitude. And POI has each time a higher effective coupling factor which is confirmed by simulation.

Quality factor is much higher for simulation than for measurements. The product $R_m(+R_s) \times C_m$ is thus supposed to be higher for measurements, it is the case. It can be explained by the fact that every loss mechanism is not introduced in the COMSOL model but only the dielectric losses.

These high quality factors in simulations induce also a high figure of merit (FoM).

Chapter 6

Sustainability

The goal of this chapter is to provide a sustainability assessment of the three different technologies of substrates for the fabrication of piezoelectric resonators which are covered in this work. The three substrate technologies are presented in section 3.5 and are summarized here :

- Bulk lithium tantalate (LiTaO_3), 42° Y-cut.
- POI (piezoelectric on insulator) which has 4 different layers (see figure 3.16) :
 - 600 nm of 42° Y-cut lithium tantalate (LiTaO_3)
 - 500 nm of silicon oxide (SiO_2)
 - 1 μm of "TrapRich" polysilicon
 - 675 μm of monocrystalline silicon (Si)
- Bulk aluminium nitride (AlN).

6.1 Method

This section outlines the method used in our work to deliver this sustainability analysis. First, the boundaries of the study will be defined. Then, the sustainability indicators used in our assessment are defined. Finally, an overview of the fabrication process of each substrate technology is presented to highlight the main primary materials required, which will then be targeted in the sustainability study.

6.1.1 Scope and assumptions

A perfect study of the sustainability of a technology is almost impossible as it would require an infinite knowledge. Indeed, it requires to know the life cycle of every device but also the impact of each device on the society and the environment. Each study is thus limited to a certain scope and it is important to define the boundaries of such a study.

In this study, the scope will be the production of wafers from raw materials such as ores. The study will focus on the production of different technologies at an industrial scale. Here, a few assumptions are made to limit the scope to the production of wafers :

- The microfabrication of the devices from the wafer (that is, the clean room process steps) is roughly the same for each substrate technology. The environmental impact of these last fabrication steps is therefore considered equal for all three technologies, and will not be covered here.
- We assume that the transformation from resonators to finite devices (which is the front end module) is performed at the same places and in the same kind of industries. The societal impact of those steps is also considered equivalent for all three technologies and therefore will not be covered in this work.

Ideally the study should be extended to the production of the final devices and their impact, but such a study would need to be the focus on a work of its own. While some concepts are borrowed from life cycle analysis (LCA), the extent of this study is nowhere near that of a proper LCA. In fact, the sustainability study presented in this work is intended to provide a basis for discussion on the use of this type of materials. Hence, a relatively wide range of sustainability aspects are covered, but the study will never go in depth into one of those aspects. To define and evaluate those aspects, various indicators are used.

6.1.2 Indicators

Here is a definition of sustainable development : "Sustainable development is development that meets the needs of the present without compromising the ability of future generations to meet their own needs." (The Brundtland Report of the World Council on Economic Development (WCED, 1987)) [63]. This definition is quite vague because sustainability is a rather complex concept. There is a need for an objective, tangible measure of sustainability. However, quantifying the sustainability aspect of a device is complicated and cannot be summarized by a single indicator.

Mike Ashby, author of the Ashby method explains that : "A corporation's ultimate success and health should be measured not just by the traditional financial bottom line, but also by its social/ethical and environmental performance". The goal is then to have a balance between three main points which are : "Planet", "Prosperity" and "People" (also called "PPP" thinking). The global "wealth" can be seen as the sum of three capitals which are : natural capital (Planet), manufactured and financial capital (Prosperity) and human and social capital (People). The objective of a sustainable technology should be to increase this global "wealth".

These three capitals are still difficult to quantify. They can be subdivided into six categories which are : "Materials, manufacture", "Design", "Regulation", "Economics", "Society", "Environment", as presented in figure 6.1.

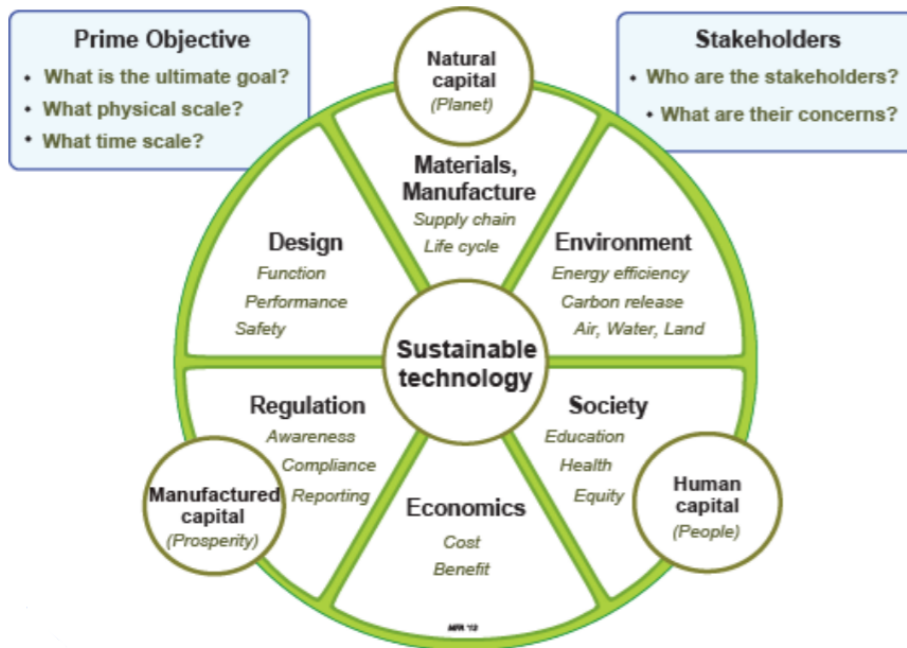


Figure 4. Necessary components of sustainable technology

Figure 6.1: Categories of sustainability indicators as presented in the Ashby method [64].

We decided to focus on a few of these categories. As we wish to highlight the impact of the technologies considered in this work, the "Economics" aspect will not be covered. Besides, the "Design" elements will not be discussed in this chapter. However, the final discussion of this thesis will combine the performance results with sustainability study results. Among the selected categories, several indicators were chosen in order for the analysis to be as objective as possible. These

Materials, manufacture	Environment
- Supply chain* - Abiotic resource depletion potential (ARDP) - End-of-life recycling input rate (EoL-RIR) - Compound Annual Growth Rate (CAGR)	- Cumulative energy demand (CED) - Global warming potential (GWP) - Water consumption - Land use
Regulation	Society
- Critical raw materials (CRM) - Economic importance (EI) - Supply risk (SR)	- Geopolitical implications* - Working conditions* - Economic equity

Table 6.1: Indicators selected for this sustainability assessment study. Qualitative indicators are marked by a star (*).

indicators are listed in Table 6.1. Each indicator is then detailed, and they are classified by the corresponding Ashby method categories they fall under.

Indicators are necessary in order to be able to objectively compare the different technologies used in this work. Values for these indicators will be looked for in environmental impact databases (such as those used for LCA) and in literature. One important thing to consider is that not all indicators give quantitative values that can be numerically compared. While many quantitative indicators are presented, we will also introduce some qualitative indicators, which will serve as basis for a discussion on the sustainability of the different technologies. Qualitative indicators are marked by a star (*).

6.1.2.1 Materials, manufacture

Supply chain :

The supply chain is not an indicator of sustainability by itself but it is important to know the main locations of extraction and processing. It will help narrowing down the scope of research for other indicators such as the working conditions and the geopolitical implications in these countries. Furthermore, it is relevant to compare the location of extraction of the ores with the location of treatment of these materials, to understand the global dynamics at play.

Abiotic resource depletion potential (ARDP) :

It is common knowledge that all resources on Earth are limited and therefore that we need to assess and monitor their usage in order to operate in a sustainable way. While there is a general feeling that there is a need for a quantification of their scarcity and their depletion rate, there is no consensus over one method of evaluation of this criterion [65].

One way to evaluate this is the Abiotic Resource Depletion Potential, introduced by Guinée and Heijungs in 1995. It is designed to address the fundamental question "How serious is the depletion of one resource compared to that of another?" and aims to express this in equivalency factors [66]. The term "Abiotic resources" refers to natural resources which are regarded as non-living. They include fossil energy resources and minerals, but exclude elements such as oxygen, hydrogen, nitrogen and carbon (only their compounds are considered). Additionally, only stock resources are considered, in opposition to flow resources such as water or solar radiation [66].

The abiotic depletion potential of resource i (ADP_i) is calculated as follows :

$$ADP_i = \frac{DR_i / (R_i)^2}{DR_{ref} / (R_{ref})^2} \quad (6.1)$$

with :

- ADP_i the abiotic depletion potential of resource i in $[\text{kg}_{\text{reference resource}} / \text{kg}_{\text{resource } i}]$ (usually the reference resource is antimony (Sb), therefore the units are $[\text{kg}_{\text{Sb}} / \text{kg}_{\text{resource } i}]$)
- DR_i is the extraction rate of resource i in $[\text{kg}/\text{year}]$

- R_i is the ultimate reserve of resource i in [kg]
- DR_{ref} is the extraction rate of the reference resource (usually Sb) in [kg/year]
- R_{ref} is the ultimate reserve of reference resource in [kg]

The ultimate reserve refers to the quantity that is ultimately available, which is estimated by multiplying the average natural concentration of the resource in the Earth's crust by the volume of the Earth's crust [66]. A high depletion potential corresponds to a scarce or over-exploited material and is therefore a sign of poor sustainability. The values for this indicator are found in the EcoInvent database using the CML-IA baseline method.

End-of-life recycling input rate (EoL-RIR) :

This indicator describes the amount of material which is recycled. More precisely, it is the percentage of end-of-life material (scrap) which is reintroduced in the manufacturing process. The computation is available at equation (6.2).

$$EoL_{RIR} = \frac{\text{Input of secondary material}}{\text{Input of secondary material} + \text{Input of primary material}} \quad (6.2)$$

Secondary material is recycled material which is used one more time in a manufacturing process. It is the opposite of primary material or virgin material which is used for the first time in the manufacturing process.

Compound annual growth rate (CAGR) :

The compound annual growth rate (CAGR) is a concept used in economics, business and investing. It is a geometric progression ratio that provides a constant rate of return over a fixed time period, dampening the effects of volatility over that period [67]. The CAGR is expressed as a percentage. It is typically used to compare the growth of a market. Here, we will use it to compare the (predicted) growth of markets corresponding to the materials that are assessed in this study. In fact, the CAGR can account for both a growth of the demand and a rise in price. As such, we consider it to be a good measure of how important and prized a material is expected to become in the coming years.

The data selected for this indicator is the data corresponding to the base material (e.g. silicon in general as opposed to silicon wafers) in order to account for other sectors using the same material. If a material is becoming extremely important and prized, we want this indicator to reflect it, even if the major contribution for this growth is not the microelectronics sector. The CAGR used in this study is a forecast for the 2021-2026 period.

6.1.2.2 Environment

Cumulative energy demand (CED) :

The energy used to fabricate an object can be evaluated through the cumulative energy demand (CED) method. Here is a description of this method : "The cumulative energy demand (CED) of a product represents the direct and indirect energy use throughout the life cycle, including the energy consumed during the extraction, manufacturing, and disposal of the raw and auxiliary materials" [68]. This indicator is expressed in [GJ/kg] or [MJ/unit] with a wafer as a unit. A high cumulative energy demand indicates a poor sustainability. The values for this indicator are found in the EcoInvent database using the Cumulative Energy Demand method.

Global warming potential (GWP) :

The global warming potential indicates the amount of greenhouse gas emitted during the fabrication of an object. In order to have a clear indicator, the quantity of greenhouse gases produced is expressed in CO₂ equivalent, via conversion factors as listed in Figure 6.2. This indicator is expressed in [kgCO₂/kg] or [kgCO₂/unit] depending on the context, with one wafer as a unit. A high global warming potential is a measure of poor sustainability.

The values for this indicator are found in the EcoInvent database using the ReCiPe 2016, Midpoint

Greenhouse Gas	Global Warming Potential (GWP)
Carbon dioxide (CO ₂)	1
Methane (CH ₄)	25
Nitrous oxide (N ₂ O)	298
Hydrofluorocarbons (HFCs)	124 – 14,800
Perfluorocarbons (PFCs)	7,390 – 12,200
Sulfur hexafluoride (SF ₆)	22,800
Nitrogen trifluoride (NF ₃)	17,200

Figure 6.2: Global warming potential of different greenhouse gases expressed in equivalent quantities of CO₂ [69].

(H) method.

Water consumption :

This indicator describes the quantity of water needed to produce the object. This can be expressed as a volume or as a mass of water per unit or per kg depending on the context. A big water consumption is a sign of poor sustainability. Furthermore, water is crucial to the microelectronics industry, which requires significant quantities of it for the fabrication of various devices such as semiconductors [70]. As such, water-use efficiency of the industry is an increasingly important challenge [71]. The values for this indicator are found in the EcoInvent database using the ReCiPe 2016, Midpoint (H) method.

Land use :

This indicator quantifies the area of land used in order to produce one object or one kg of an object. It is expressed in square meters of equivalent area of crops used for one year [m²a crop-eq]. A big land use indicates that a lot of land is used to produce a small quantity of material. This is a sign of poor sustainability because this land could be used for another purpose. The values for this indicator are found in the EcoInvent database using the ReCiPe 2016, Midpoint (H) method.

6.1.2.3 Regulation

Critical raw materials (CRM) :

Since 2011, a list of critical raw materials (CRM) is published by the European Union (EU) and is regularly updated (the most recent version being that of 2020, shown in Figure 6.3). These materials are considered crucial for the EU economy and associated with a high risk for their supply [72]. A raw material is defined as a CRM if it exceeds certain thresholds (defined by the EU) related to: (1) Economic Importance (EI) and (2) Supply Risk (SR) (as illustrated in Figure 6.4. The thresholds are 1 for SR and 2.8 for EI [72]. The data used to compute these indicators is averaged over the last 5 years. The method used to determine this list is detailed in Appendix G. This list is not a ranking of the most critical materials. It is rather an enumeration of the materials considered as critical in 2020. Therefore, the output of this indicator is binary, as a material can either be present on this list or not. Most primary materials compared in this study are present in this list. In order to evaluate the criticality of those materials, the two quantifiable indicators implicitly used to define this list (EI and SR) will be considered as quantitative indicators in this study.

Economic importance (EI) :

2020 critical raw materials (new as compared to 2017 in bold)		
Antimony	Hafnium	Phosphorus
Baryte	Heavy Rare Earth Elements	Scandium
Beryllium	Light Rare Earth Elements	Silicon metal
Bismuth	Indium	Tantalum
Borate	Magnesium	Tungsten
Cobalt	Natural graphite	Vanadium
Coking coal	Natural rubber	Bauxite
Fluorspar	Niobium	Lithium
Gallium	Platinum Group Metals	Titanium
Germanium	Phosphate rock	Strontium

Figure 6.3: List of the critical raw materials in 2020 [73]. The most recent additions to this list are written in bold.

The EI indicates the importance of a material for EU economy. It is computed as follows :

$$EI = \sum_s (A_s * Q_s) * SI_{EI} \quad (6.3)$$

Where :

- EI is the economic importance
- A_s is the share of end use of a raw material in a sector.
- Q_s is the sector's value added.
- SI_{EI} is the substitution index of a raw material related to economic importance.
- s denotes the sector. The different sectors are defined by the NACE Rev. 2 classification [74].

A detailed description of the parameters used to compute this indicator is available in Appendix G.

Supply Risk (SR) :

Supply risk accounts for the risk of disruption in the European supply of a material. It is measured at the "bottleneck" stage of the supply chain, which is the stage with the highest risk. It is usually taken as the extraction stage, unless processing proves to present a higher risk of disruption. Two sets of producing countries are considered : global suppliers on one hand, and countries that supply the EU on the other hand (including EU countries themselves). It is calculated following equation G.3.

$$SR = \left[(HHI_{WGI,t})_{GS} \cdot \frac{IR}{2} + (HHI_{WGI,t})_{EU_{sourcing}} \left(1 - \frac{IR}{2} \right) \right] \cdot (1 - EoL_{RIR}) \cdot SI_{SR} \quad (6.4)$$

where :

- SR is the supply risk
- $HHI_{WGI,t}$ is the Herfindahl-Hirschman Index, taking into account the World Governance Index WGI and the trade parameter t adjusting WGI . GS denotes global suppliers, while $EU_{sourcing}$ denotes countries that are actual supply sources for the EU
- IR is the import reliance
- EoL_{RIR} is the end-of life recycling input rate
- SI_{SR} is the substitution index related to supply risk

A detailed description of the parameters used to compute this indicator is available in Appendix G.

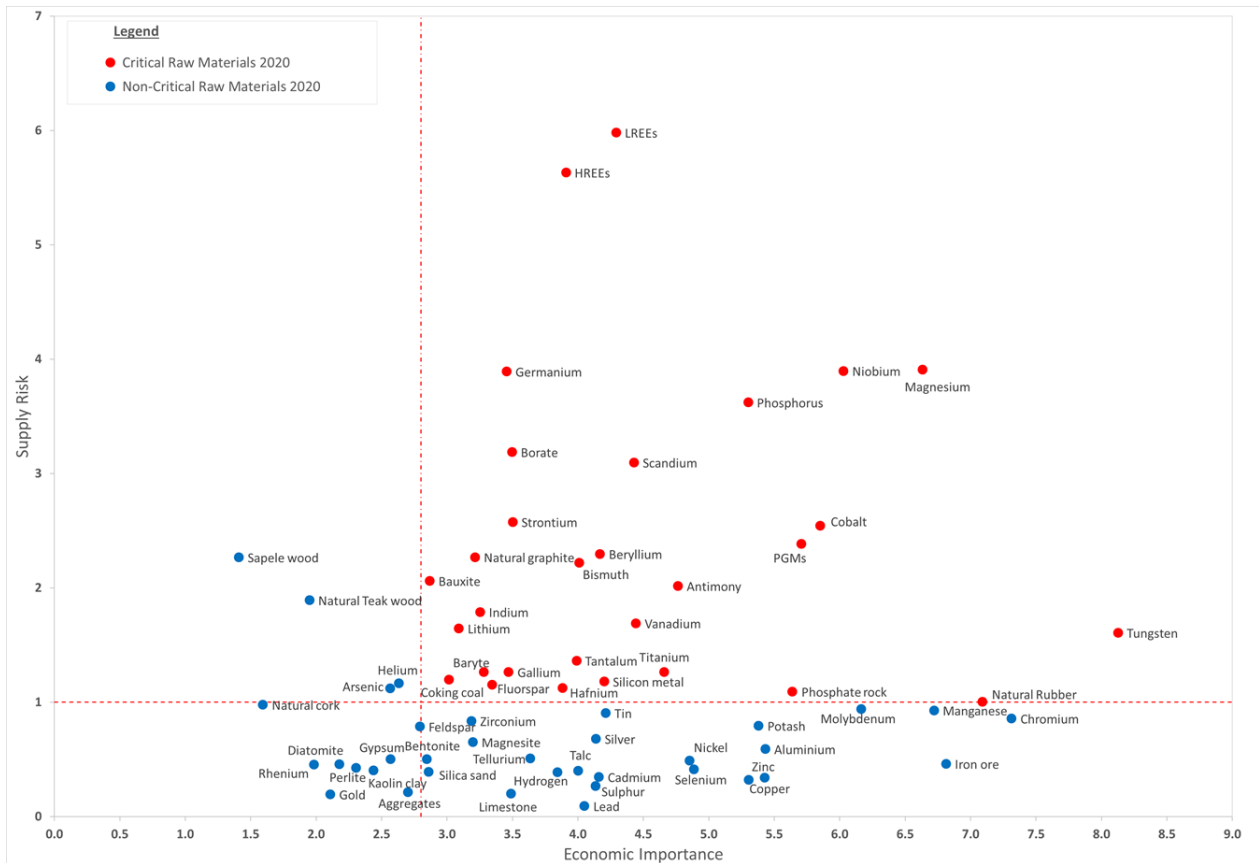


Figure 6.4: CRM classification with thresholds for EI and SR

6.1.2.4 Society

Geopolitical implications :

The geopolitical implications associated with the production of a device are evidently impossible to quantify. However, their importance in the context of the extraction of some minerals can simply not be overlooked. This qualitative indicator will serve as basis for a discussion about the conflicts and issues which are closely linked to the extraction of minerals.

Working conditions :

The working conditions fall into the category of indicators that are not quantified, but that are simply impossible to leave out, such is their moral importance. Indeed, the working conditions of workers at the very beginning of the supply chain, such as in mines, are often extremely tough. With health problems, human rights violation and child labour reported in some cases. Hence the comparison of working conditions is particularly relevant at the extraction step. Steps further down the supply chain, such as the treatment and fabrication of wafers, are realized in the same kind of industries for each technology, and we can assume there is therefore little difference in working conditions at that stage of the supply chain.

Economic equity :

This indicator answers the need for a quantifiable indicator of the social impact of the production of a given device. It is taken as the ratio between the average salary of a worker and the average salary in the country. Here, the term "worker" designates people working at the very beginning of the supply chain, which in this context are usually miners. The workers which work for the extraction of the ores are the ones who are the most exploited and whose salary is the lowest of the supply chain. Simply comparing the salaries of people working in different countries makes little sense, as the cost of living and the socio-economic conditions can greatly vary from one country to another. As such, we defined the economic equity as the ratio between worker salary and average salary in

the country. The gross national income (GNI) per capita is taken as a proxy for the average salary. The GNI is converted to U.S. dollars using the World Bank Atlas method, and is then divided by the midyear population [75]. For this indicator, a higher value is naturally desirable as it means a better salary for the workers at the beginning of the supply chain.

$$\text{Economic equity} = \frac{\text{Worker average salary}}{\text{GNI per capita}} \quad (6.5)$$

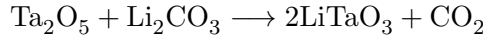
6.2 Fabrication Process

Because the scope of the sustainability extends from the primary material extraction to the wafer fabrication, it is relevant to know how to go from one stage to the other. The objective is to identify the key materials involved in the fabrication process, in order to target those materials are the subject of the study. This section presents the different steps from ore to wafer for each technology.

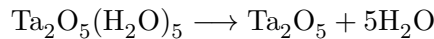
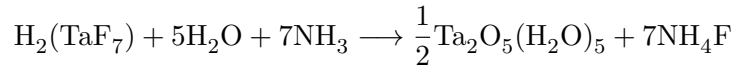
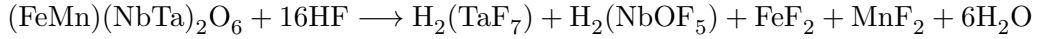
1. Primary ores extraction
2. Reactions to obtain the compound of interest (intermediate or final product)
3. Monocrystalline growth process and slicing

6.2.1 Lithium tantalate

Lithium tantalate (LiTaO_3) is usually synthetized by sintering of tantalum pentoxide (Ta_2O_5) and lithium carbonate (Li_2CO_3), both in the form of small solid pellets [76][77].

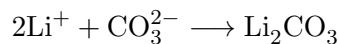
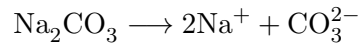


Let us now investigate the production of those two components. Tantalum pentoxide is obtained from tantalite which is contained in coltan (short for columbite-tantalite). Here are the reactions corresponding to the refining of tantalum pentoxide (Ta_2O_5) from tantalite ($(\text{FeMn})(\text{NbTa})_2\text{O}_6$) [78]:



The other reactant to produce lithium tantalate is lithium carbonate (Li_2CO_3). It can be obtained by different ways :

- From brine (water with a high concentration of salt) in salars (salt lakes), which have a lithium concentration of 0.06% to 0.15% [79]. Brine first goes through solar evaporation steps, which increase the lithium concentration to up to 6%. Then, it has to be treated to remove unwanted contaminants such as magnesium and bore. Then finally the desired lithium carbonate (Li_2CO_3), lithium chloride (LiCl) and lithium hydroxide (LiOH) can be produced [79]. Lithium carbonate (Li_2CO_3) is usually precipitated with the addition of carbonate (CO_3^{2-}), which reacts with the Li ions from brine. In many cases, sodium carbonate (Na_2CO_3) is used, which gives the following reactions [79] [80]:



- From lithium-bearing ores, which usually require comminution (reduction into smaller pieces) and beneficiation (refining) to produce concentrates containing 4 to 6 % of Li_2O . Those concentrates are then roasted and leached to extract a lithium-rich solution. This kind of solution is then treated similarly as brine, mainly by precipitation to produce lithium compounds (Li_2CO_3 , LiCl and LiOH) of chemical or battery grade [79].

Spodumene ($\text{LiAl}(\text{SiO}_3)_2$) is the main mineral that has been commercially processed to produce lithium compounds [79]. To produce Li_2CO_3 from spodumene, the mineral is put through the following process [81]:

1. Grinding to a powder
2. Calcining at 1100 °C
3. Treatment with sulfuric acid (H_2SO_4) at 250 °C
4. Solvation with water to extract Lithium Sulfate (Li_2SO_4)
5. Separation of Aluminium Sulfate ($\text{Al}_2(\text{SO}_4)_3$)
6. Precipitation of Li_2CO_3 with soda ash (sodium carbonate, Na_2CO_3)

6.2.2 POI

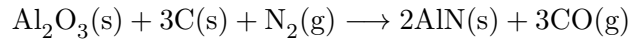
The first steps of the production of POI wafer technology are the same as in the previous section. Indeed, the POI wafers are fabricated using a wafer of lithium tantalate, by the "Smart-cut" process which is described in section 3.5. The POI wafers fabricated this way are supposed to contain much less lithium tantalate than a bulk wafer. Still, it is relevant to investigate their sustainability. Silicon is the major part of the wafer in this case. Silicon does not exist under its pure form Si naturally. But it can be found in quartz form, also called silica sand (SiO_2). Si can then be extracted as follows :



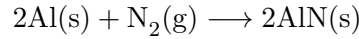
6.2.3 AlN

There are 2 ways to synthetize the aluminium nitride which is used at industrial scale [82] :

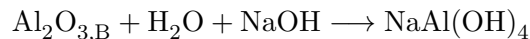
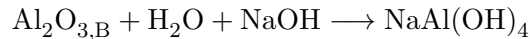
- From alumina (aluminium oxide) :



- From pure aluminium :



The ore which is used in order to obtain aluminium is bauxite. Bauxite is the main source of aluminium [83], it contains alumina (or aluminium oxide) Al_2O_3 , gibbsite ($\text{Al}(\text{OH})_3$) and other compounds. Alumina can then be produced from bauxite thanks to the Bayer process [84]:



Indice B indicates compounds which come directly from bauxite and are thus not pure. After this reaction, residues can be separated thanks to a sedimentation process [85]. Then pure alumina is recovered via a precipitation process :





2 tons of alumina can be obtained from 4 or 5 tons of bauxite depending on the quality of bauxite. Then 1 ton of aluminium can be obtained from the two tons of alumina with an electrolytic reduction: at an aluminium smelter, alumina is poured into special reduction cells with molten cryolite at 950°C. Electric currents are then induced in the mixture at 400 kA or above; this current breaks the bond between the aluminium and oxygen atoms resulting in liquid aluminium settling at the bottom of the reduction cell [86].

6.3 Results

Table 6.2 summarizes the results obtained for each previously defined indicator. The main materials considered in the study are selected based on the fabrication processes outlined in section 6.2. The four materials considered are : lithium, tantalum, silicon and aluminium. While some indicators from the "Materials, manufacture" category often use data that is based on the most general definition of the materials, in most cases specific stages of those materials are considered.

For LCA-derived indicators such as ARDP and "Environment" indicators, data closest as possible as the wafer material was used: "Lithium carbonate" for lithium, "Tantalum, powder, capacitor-grade" for tantalum, "Silicon, single crystal czochralski process, electronics" for silicon, "Aluminium, primary, ingot" for aluminium.

In the supply chain section, two stages of the material are considered: the extraction stage and the processing stage. In the case of silicon and aluminium, their extraction stage material is the primary material, respectively silica sand and bauxite. These primary materials are also considered in the "Regulation" category indicators. Finally, "Societal Impact" indicators also consider the extraction stage of materials only, with a focus on the mining of lithium, coltan (for tantalum), silica sand and bauxite.

6.3.1 Qualitative indicators results

In this section, explications for the qualitative indicators are provided.

6.3.1.1 Supply Chain

Lithium :

The main producers of lithium (at extraction stage) are Chile (38%) and Australia (36%). The main exporters of lithium at processed stage are Chile (44%) and China (39%) [87]. Lithium from Chile comes from brine, while lithium from Australia comes from hard rock mining, mostly of spodumene [108].

Tantalum :

The tantalum supply chain is obviously strongly connected to coltan as it is the ore from which it comes. The main global tantalum producers are the Democratic Republic of the Congo (33%) and Rwanda (28%) [87]. However, Rwanda is one of the top exporters of coltan despite having not having the mines that match this production, leading to many accusations of looting and exploitation of coltan by Rwanda in DRC [109] [110].

Silicon :

The main producers of silica sand are the USA (38%) and the Netherlands (17%), while the main producer of silicon metal at processed stage is China (66%) [87].

¹Data gathered from Ecoinvent.

²Controversial as Rwanda is accused of looting coltan from DRC. While the CRM list attributes a similar share to the two countries, the US Geological Survey lists DRC as the top producer, with almost triple the production of Rwanda [88].

³Not listed as main producer in the CRM list [87], but cited as top producer by the US Geological Survey [88].

Indicator	Lithium	Tantalum	Silicon	Aluminium	Sources
Materials, manufacture					
Supply Chain (Extraction)	Chile (38%), Australia (36%)	DRC (33%), Rwanda ² (28%)	(Silica sand) USA (38%), Netherlands (17%)	(Bauxite) Australia (28%), China(20%), Guinea ³	[87][88]
Supply Chain (Processing)	Chile (44%), China (39%)	unavailable data	(Silicon metal) China (66%)	(Aluminium) China (52%)	[87]
ARDP [kgSb-eq/kg]	2.27 e-5	0.0018	1.24 e-4	4.91 e-5	¹
End-of-life recycling input rate	0%	0%	0%	12%	[87]
CAGR	10%	6%	6.1%	4%	[89][90] [91][92]
Environment					
Cumulative energy demand [GJ/kg]	0.0326	4.47	4.73	0.162	¹
GWP [kgCO ₂ -eq/kg]	2.26	290	234	9.72	¹
Water consumption [m ³ /kg]	0.0436	2.83	29.7	0.241	¹
Land use [m ² a crop-eq/kg]	0.166	53.3	6.46	0.0847	¹
Regulation					
Critical Raw Material	Yes	Yes	Yes (Silica sand: No)	No (Bauxite: Yes)	[87]
Economic importance	3.1	4.0	4.2 (Silica sand: 2.9)	5.4 (Bauxite: 2.9)	[87]
Supply risk	1.6	1.4	1.2 (Silica sand: 0.4)	0.6 (Bauxite: 2.1)	[87]
Society					
Geopolitical Implications	Political issue, harm to local population	Armed conflicts, criminality, political issue, harm to local population	Criminality	Harm to local population	[93][94] [95][96] [97][98] [99][100]
Working Conditions	Standard	Violence, abuse, child labour, health risks	Standard	Health risks	[96][97] [98][100]
Economical Equity	Chile: 1.001 - 1.008, Australia: 1.099 - 1.321	DRC: 0.945 - 4.727	USA: 0.595, Netherlands: 0.922 - 1.168	Australia: 1.099 - 1.321, China: 1.414	[96][97] [98][75] [101][102] [103][104] [105][106] [107]

Table 6.2: Indicator results

Aluminium:

The main producers of bauxite are Australia (28%) and China (20%) with China being the main global processor of aluminium, too (52%) [87]. While the CRM assesment of the EU does not list

Guinea as one of the top producers of bauxite, other reports such as the US Geological Survey [88] do.

6.3.1.2 Geopolitical implications

Tantalum is labelled as a conflict mineral, which are minerals coming from politically unstable areas, where the minerals trade can be used to finance armed groups, fuel forced labour and other human rights abuses, and support corruption and money laundering. The term 3TG is used to refer to tin, tungsten, tantalum and gold, which are notorious conflict minerals [111]. The concept of conflict resource is also extended to other natural resources [112].

Lithium mining :

Although lithium is not commonly listed as conflict resource, it is sometimes labelled as such, because of ongoing and possible future problems around its extraction, especially in the so-called "lithium triangle", a region of the Andes known for its lithium reserves. The lithium triangle is at the intersection of Bolivia, Chile and Argentina, which are the top three countries with the most lithium resources [88]. However, this potential is only partly exploited as of now, with Bolivia for example not among the top producers.

Lithium extraction is at the center of both local and international political tensions in all three countries of the lithium triangle. In Chile and Argentina, local communities are resisting lithium mining as it poses a threat to their lives and to the ecosystem, with shortages of water associated with lithium mining mentioned [94] [95]. In Bolivia, where the majority of the lithium extraction potential is still untapped, it has become a major topic of politics, with some accusations of it being the reason behind the USA's support for the overthrowing of the previous government [93]. In all cases, the population from these countries is, perhaps rightly, concerned that they will not benefit from this exploitation, with most profits going to foreign multinationals.

Tantalum (coltan mining) :

Minerals in Democratic Republic of Congo have been at the center of ongoing conflicts since the beginning of the century. Wars between 1996 and 2003 have been especially violent and are estimated to be one of the deadliest conflicts in the world since World War 2. The deaths are not necessarily directly due to violence, but also from the diseases and starvation associated to and exacerbated by war [113].

Its origin being closely tied to the Rwandan genocide, this war has been funded by the lucrative trade of minerals, including coltan. The extraction is done both legally and illegally, by "artisanal" miners who use picks, shovels and sometimes their bare hands to dig it out. Migrants and children make up a big part of these miners, and working conditions are predictably atrocious, with exposition to toxic dust, heavy metals and dirty water with little to no equipment or medical services.

Participation in these conflicts by foreign companies has been documented, notably by the UN. Those companies worked hand in hand with military groups or local militias, in order to benefit from the precious minerals.

This war economy has set the tone for mining conditions in DRC throughout the 21st century. The profitability of tech products involving tantalum is intrinsically linked to the brutal way the mineral is extracted in DRC.

Over the years, attention has been brought to these highly problematic practices, and there has been attempts to provide more transparency, traceability and ultimately to hold responsible organizations accountable. This task is very complicated, almost impossible. Indeed the mines validated as conflict-free can be just a few hills away from those controlled by armed groups. The trade is messy, with miners and mineral traders operating independently and constantly on the move across the region. Conflict minerals can easily leak into the supposedly clean supply chains [97].

Success for these initiatives was mixed, however, as in some cases the measures put in place were rather an embargo, which only led to further control for armed groups, and further distress for the workers.

To avoid this embargo and the fact that coltan is not exported anymore from DRC, a company

so-called MMR was created. MMR is a pioneer in the supply of untained materials. Its first client are companies like Fairphone or Motorola which want untained coltan. Even if it is a good idea, this company is a complete monopoly and has exclusive rights to purchase the entire production of the four main artisanal mines in what was formerly Katanga Province. Following a MMR employee : “We don’t set prices. We impose them on miners.” [97]. And the price of MMR is really cheaper than the one of other trader (22\$/kg vs 50 \$/kg). And none of the members of the price-setting committee effectively represents the miners’ interests. Knowing that coltan miners are working as much as 12hours a day in hard condition in order to help their family survive [98], we understand easily that this monopoly which pay them less than other traders is not the best solution and push them to sell it to mineral traders.

The situation does not look like progressing that much, as the same old mechanisms of dominance and exploitation of African resources by western countries and companies are ongoing, keeping the vast majority of DRC in poverty, while its riches are being taken from the ground.

Silicon (silica sand mining) :

Even though the share of silica sand used for silicon production is minimal, with other uses such as construction and glass being the majority [87], it is worth mentioning that sand extraction is harmful in many ways, including from a social impact point of view. Indeed, illegal mining of sand occurs in many places in the world, where criminal gangs manage the mines, with exploitation, killings and child labour part of the associated problems [99].

Aluminium (bauxite mining) :

Similarly to Bolivia with lithium, Guinea possesses the world’s biggest bauxite reserve, although it is not living up to its production potential yet [88]. In a way that is becoming quite familiar, foreign companies (in this case, from Russia and China) are reaping the benefits of bauxite mining, with too little profit going to Guinea, partly because of its lack of refining facilities for alumina production [114] [115]. Furthermore, reports the consequences of bauxite mining on human rights highlight concerns for local populations’ rights, health, land and access to clean air and water [100]. The report also cites communities angry at the lack of positive consequences the booming bauxite mining sector induces for them.

6.3.1.3 Working Conditions

Tantalum (coltan mining):

Coltan is mined the same way gold was mined in 1800. It is mined by hand. People fill bucket of mud and water and coltan sink to the bottom because it is heavier [96]. Conditions of work are terrible, Coltan is extremely heavy, workers are exhausted heat is intense and this work is done in the mud with all the diseases, dirt and animals which live there.

Furthermore a lot of people which work in the mines are children. Child labour in coltan mining is well known. They start working at a young age like 11 years or even younger [98].

The average income of a Congolese worker does not provide a sufficient income to sustain a family [116]. Many workers in DRC earn less than 10\$ a month. A coltan miner, however, can earn between 10 and 50\$ a week and is able to sustain his family. That is exactly why people there want to work in coltan mines. But the work is worth at least the salary given the fact that miners work up to 12 hours a day without any days off. A lot of mines are ruled by armed militias, which is obviously stressful.

There are also cases of sexual abuse in this context. In this article [98], a women explained her boss told her that she has no sex with him he would drive her out of the mine zone. She was punished for refusing, her jobs became thus more and more difficult, her and her child were suffering thus she agreed. A lot of women are abused while working in the mines but solution are limited.

Lithium mining:

Lithium extraction from brine and minerals are both automatized with an established process flow [117]. Workers are therefore rather mining engineers or operators, with seemingly good working

conditions.

Silicon (silica sand mining) :

Silica sand mining appears to be performed with automatized mining equipment [118]. In that case, workers are rather operators than miners. The conditions therefore seem decent.

Aluminium (bauxite mining) :

Although mentions of manual work exist [119], most bauxite mining is performed with machinery [120]. Hence, workers are rather operators than miners. They are however reports of health concerns for people working or living around bauxite mining sites, with respiratory issues a notable problem [100].

6.3.2 Results for one wafer of each technology

As explained in the beginning of this chapter, the functional unit of our sustainability study is a wafer. Therefore, we need to convert the data we obtained for a kilogram of material. Furthermore, we want to account for the amount of lithium, tantalum, silicon and aluminium that are contained in a wafer of bulk lithium tantalate, POI or aluminium nitride. In order to achieve that, we will look at the chemical reactions (presented in section 6.2 necessary for the production of wafer material, and weight the contribution of different elements by using their molar mass. The calculations are briefly outlined here.

- Lithium tantalate (LiTaO_3) contains 85.7% (in mass) of tantalum oxide (Ta_2O_5) and 14.3% of lithium carbonate (Li_2CO_3). The data gathered in Table ?? from Ecoinvent are coming from lithium carbonate databases in the case of lithium, and "tantalum powder, capacitor grade" in the case of tantalum. As such, we can take the lithium carbonate values directly. However, in the case of tantalum, we made the assumption that the tantalum powder was in fact tantalum oxide, as it is used in capacitors.
- For the POI technology, we also based our computations on a few assumptions. First, the amount of lithium tantalate required was assumed to be equal to the lithium tantalate volume fraction inside a POI wafer. Besides, we neglected the contributions of the silicon oxide and polysilicon layers, considering them as silicon. Then, we used the densities of lithium tantalate and silicon to compute their mass fraction inside a POI wafer. As a result, POI is composed of 0.088% of lithium tantalate, and 99.112% of silicon. LT data was directly taken from the calculations of the previous point, while silicon data from Ecoinvent comes from "silicon, single crystal czochralski process, electronics" which is precisely the type of silicon used here and therefore needs no transformation.
- The aluminium nitride case is the most straightforward. As aluminium data from Ecoinvent comes from the "aluminium, primary ingo" database, we considered it valid for Al. A conversion to AlN was required using the reaction equation, with the impact of nitrogen neglected. AlN contains 98.1% (in mass) of aluminium, and 1.9% of nitrogen.

Table 6.3 shows the results for each technology. Only the five indicators which strongly depended on the quantities of material were taken into account here. The other indicators are more qualitative or are defined more generally (e.g. lithium as a whole sector is considered, as opposed to only lithium carbonate), and are therefore not repeated here. The mass fraction of each element can help understand the impact of each technology for qualitative indicators, however, due to the nature of social impact or regulation indicators, no weighting based on material quantity was possible.

As a summary, we can observe that tantalum has a big contribution in the lithium tantalate impact, that the POI is almost entirely composed of silicon, and the impact of aluminium is a very good approximation for the impact of aluminium nitride.

Then, a second table, this using a single wafer as a unit, was produced (6.4. The reference wafers are considered to be 150 mm wafers, with a thickness of 675 μm . Those are standard dimensions

used in the industry. It is worth noticing that the indicator units have been modified to provide a more easily understandable value.

Indicator	Lithium tantalate	POI	Aluminium nitride
Materials, manufacture			
ARDP [kgSb-eq/kg]	1.69 e-3	1.28 e-4	3.23 e-5
Environment			
Cumulative Energy Demand [GJ/kg]	4.192	4.728	0.107
Global warming potential [kgCO ₂ -eq/kg]	271.99	234.11	6.40
Water consumption [m ³ /kg]	2.658	29.623	0.159
Land use [m ² a crop-eq/wafer]	49.950	6.584	0.056

Table 6.3: Quantitative indicator results

Indicator	Lithium tantalate	POI	Aluminium nitride
Materials, manufacture			
ARDP [mgSb-eq/wafer]	150.34	3.59	1.25
Environment			
Cumulative Energy Demand [MJ/wafer]	373.02	132.03	4.14
Global warming potential [kgCO ₂ -eq/wafer]	24.203	6.537	0.248
Water consumption [l/wafer]	236.48	827.12	6.16
Land use [m ² a crop-eq/wafer]	4.4448	0.1838	0.0022

Table 6.4: Quantitative indicator results

6.4 Interpretation of the sustainability study

Sustainability cannot be assessed by a single criteria. Hence, a series of indicators have been selected, ranging from materials and manufacture, environment, regulation and society related indicators. Such is the nature of these indicators, it is impossible to compare them, let alone weigh or classify them. As such, no definitive conclusion can be reached on which technology is the more favorable from a sustainability point of view, as it would mean hierarchizing the various aspects of sustainability. Nevertheless, some observations can be made for each category of indicators.

Looking at the supply chain, some interesting dynamics can be noted. The main countries involved in the extraction and the processing of a material are often different, which implies that the extracting countries are selling the primary material to the processing countries. Processed materials usually boast a higher value, which means that processing countries make a bigger profit than extracting countries. It is worth mentioning that the extraction tends to take place in developing, southern hemisphere countries, while the processing tends to take place in developed, northern hemisphere countries. This illustrates the global dynamic of the material economy, where countries possessing the valuable ores end up earning only a small share of the benefits, while countries exporting a product with added value after processing reap large profits.

The ARDP is highest for tantalum, meaning that producing a kg of tantalum contributes more to resource depletion than for other materials. Even though a large ARDP does not necessarily mean that a resource is scarcer than others, it is of course a factor that can influence this indicator. Besides, even though lithium currently has the smallest associated ARDP, it has the highest CAGR,

meaning that the lithium market is expected to grow significantly in the coming years. While this might not be a surprise considering the recent boom in other lithium sectors such as batteries for electrical vehicles, it indicates the fact that the picture could change drastically in the coming years. Indeed, the impact of lithium extraction on resources could be strongly aggravated if the demand keeps on growing as it is.

As far as recycling is concerned, we can observe that lithium, tantalum and silicon offer none or almost no recycling possibilities, while aluminium is a material well-known for its recyclability. However, it has to be noted that these are the numbers for aluminium, not aluminium nitride, whose recycling is not documented. That being said, we can consider that from a manufacturing point of view, aluminium looks most favorable.

Environmental indicators can be assessed mainly through Table 6.4, which gathers values for a single wafer as functional unit. As the bulk lithium tantalate technology is the one using the most tantalum and lithium, it is logically the one with the biggest environmental impact. Indeed, it has the highest resource depletion potential, energy demand, global warming potential and land use among the three substrate technologies. POI scores better, but silicon production requires enormous quantities of water. Aluminium nitride seems to be the option with less impact on the environment, in light of these indicators.

As all material options are listed in the critical raw material list under some form, it is useful to look at economic importance and supply risk. We can observe that a material usually has a very high EI or a SR value, but rarely a high value for both these indicators. This makes conclusions hard to draw as it is difficult to weigh one of those indicators above the others. However, it is important to keep in mind that as all those materials are critical, no wafer technology presented here can be considered as the perfect solution.

Research about the societal impact of the extraction of those materials have allowed us to gain insight into the conditions in which it is operated. Often, a quick search on the internet is enough to find reports and articles relating the human, social and political problems associated to some of the mining practices associated with the extraction of these materials. Coltan, the primary ore for tantalum, stands out as an incredibly problematic material. The abysmal violence and human disasters around coltan mining is the norm, not the result of a few exceptions. The situation is such that coltan mining is impossible to dissociate from war in DRC and Rwanda, rightly earning the "conflict mineral" label to tantalum. We found out that efforts had been made from some companies to try to establish more transparent, ethical supply chains for coltan. However, reports show that in practice, this is far from being the case, and that virtually all the coltan used today is associated with these problems. Lithium, too, is the source of many human and political problems. Albeit less violent than in the case of coltan, the issues surrounding lithium mining are a real concern, especially considering the lithium economy is tipped to continue to explode in the coming years. This draws a very dark picture for lithium tantalate, which is undoubtedly the most problematic substrate technology option among those studied, from a social point of view. Mentions of trouble around some silica mines exist, so do health concern reports about bauxite mining site workers. However, those issues seem easier to address than the complex geopolitical implications of coltan or lithium mining. Nevertheless, in the case of bauxite mining in Guinea, reports highlight the strong influence of foreign companies, and the growing angst of the local communities towards these Western or Asian companies which make significant profits, while Guinea itself only receives a limited share of the benefits, not to mention that communities surrounding the mines often only experience the negative side of it. A similar pattern is observed with lithium in Bolivia, which despite being aware of the rich lithium reserves it possesses, seems to have found no other solution than dealing partnerships with Western countries to start lithium mining projects. The resulting limited benefits for the country and harm to the people and the environment have understandably sparked discontent, and lithium mining has become an extremely important political topic in recent years.

The recurrent pattern of developed countries exploiting the large amount of resources of devel-

oping countries, often neglecting or even fueling the associated human, social and environmental problems in those countries, is concerning, and begs for a general questioning of the current global economic and industrial practices.

Chapter 7

Discussion

From a performances point of view, it seems rather clear that POI technology is the most suitable technology for SAW resonators among those studied in this work. The higher coupling factor allows for a larger filter bandwidth, and the higher quality factor (than bulk LT and AlN) leads to steeper skirt. The TCF is the lowest due to the different layer (LT, SiO₂, Si) and it can be reduced by properly adjusting the thickness of different layers. Furthermore, the phase velocity being slightly faster in POI than in bulk LT, it allows to increase the upper limit of the frequency range usable by SAW technology, with the same lithography accuracy.

Some things can be noticed regarding AlN: its phase velocity is much higher than the leaky wave in LT (either in bulk LT or POI), and can therefore extend the range of frequency of SAW. No clear conclusion can be done regarding the quality factor since only simulations were realized (and did not contain all the losses mechanism), but combining simulation and literature, it is reasonable to think that the quality factor is in the same order of magnitude or even higher than the quality factor for LT technologies. However, its coupling factor is so weak that this technology does not seem as suitable as LT and especially POI for SAW resonators.

The figure of merit (FoM) of POI resonators is clearly the highest, which translates the fact that this technology is the best choice for SAW technology, among the three that we presented in this work.

It is necessary to keep in mind that other techniques can be used to obtain higher coupling factors for AlN [32], even though it does not reach the values of LT. Furthermore, other technologies (lamb wave, BAW,...) using AlN seem promising to accomplish the same functions as SAW resonators ([31] [47] [46]). Those other technologies are not covered here as this work focuses on SAW resonators.

From a sustainability point of view, we observed that none of the three technologies presented in this work is perfectly clean, as all materials used are considered as critical under some form involved in the wafer fabrication process. Furthermore, whereas some indicators offer a very objective mean of comparison, others are simply impossible to quantify. Besides, it is very difficult to consider an indicator as more important or less important than another, such is their diversity. Nevertheless, some observations can be made, and some key elements particularly stand out. In the course of our sustainability study, we identified the primary materials, mostly ores, from which the wafers were produced. Researching information about the extraction of these primary materials very quickly brought a lot of concerning reports to light. Coltan mining, in particular, stood out as intrinsically linked to extremely complex and alarming conflicts. War and coltan mining seem tangled in a way that almost seems beyond repair, as this connection is decades old and efforts to stop it have bore very little fruit until today. This clearly justifies the "conflict mineral" label that tantalum has, and therefore strongly encourages the avoidance of the use of lithium tantalate. The case of lithium tantalate is not helped by the fact that lithium, too has its own toll of present, and anticipated future problems. The recent demand for this material sparked a rapid upscaling of its extraction, leading to the deterioration of the environment, the threat to the living conditions of local communities, and associated geopolitical complications. As lithium tantalate seems problematic both socially, politically and environmentally, the other technologies naturally appear more favorable. Silicon, the main

constituent of POI, albeit being conflict-free and abundant, still has a non-negligible environmental toll. Aluminium, the main constituent of AlN, seems a much more sustainable material, although reports about the mining of its primary material, bauxite, raise human condition concerns in some parts of the world. In that regard, POI and AlN seem more favorable options than bulk lithium tantalate, but we have to keep in mind that they are no panacea.

Aurélien Barrau said : "Decreasing our energetic consumption is not enough. It is necessary but it is not enough. We claim that we must use the available energy adequately. But it is possible to devastate cheerfully with little energy... We can raze the forest with bulldozers working with solar energy : the carbon footprint is good but the act remains dramatic. [...] If it is about saving the industrial civilisation as it is existing, the struggle makes no sense, has no interest." [121]

A comparison with our work can be done here. Finding solutions to decrease our coltan and critical materials consumption, or even completely stopping it, with the aim to meet the requirements of 5G and pushing the progress in that way is completely comparable to razing the forest with solar bulldozers. We are using less damaging technologies leading to the same solution, a world where living is becoming increasingly difficult. We know exactly what is happening and what is coming. We know the increasing harvesting of energy and resources means sacrifices and suffering for a lot of living beings, human or not. This explanation corresponds more to the use of AlN to replace LT. In our sense, POI is even worse. To come back to the solar bulldozers metaphor, it is like using a solar bulldozer to raze the forest because it is more efficient than the bulldozer working with fuel. We are using something less damaging, without any privation or awareness, to go even faster towards this abject world.

Furthermore, as Soitec never mentions the sustainable aspect when they talk about POI substrate, only citing the efficiency, we could easily believe that reducing their coltan consumption was not their goal. It is worth wondering how these POI substrates are fabricated. If the company really understands the problem concerning this material and if the treatment of it is adapted to reduce its consumption as much as possible.

Chapter 8

Conclusion

Having been through the whole process of this work, we can reflect on its objective, which was detailed at the beginning. The aim of this work was to study selected technologies used for SAW resonators (LiTaO₃, POI, AlN) in order to provide a documented insight on which of these technologies is the most suitable for future SAW resonators, from both a performance and sustainability point of view. While a definitive answer to this question was not reached, we offered guidelines based on various criteria. In fact, the conclusion of this study strongly depends on the value we attribute to its different aspects. Some will give the performances the biggest importance, and consider the POI as an excellent alternative to conventional bulk LT. The sustainability advantages of AlN might appeal to others and influence their research or investment towards it, despite seemingly lower performances. Generally speaking, today's industry and academical world would lean towards the first option, privileging performances. While this reasoning makes sense, we consider that fails in considering the context in we live in. Every single one of us has had more than enough reminders that the way of living that is dominant in the 21st century is clearly unsustainable, and is beginning to visibly takes its toll on the environment and on the living. Inequalities are aggravated, places are destroyed, lives are crushed in name of progress. We feel that in such context, the definition of progress has to shift. It can no longer be blindly equaled to growth, profit and performance. We deeply believe that decreasing social inequalities and mitigating the destruction of the environment should be the driving forces of any attempt at progress.

The sustainability study conducted in this work is far from being complete or definitive. However, we would wish to see such studies being included in the works we encounter in the literature. Taking into accounts social and environmental aspects should be systematic, not anecdotic. In the realization of this work, being surrounded by people pushing us to embrace such aspects has greatly enhanced our motivation. As this work embodies the end to our engineering studies, we wish is to carry this approach into our careers and lives. The truth is, we are not satisfied with the second possible interpretation we suggested either. We feel that if our learnings of this work are that AlN is the way to go because of its improved sustainability compared to other technologies, we are all wrong. Reading, looking, researching about the impacts of those technologies made us want to push the reflection beyond the choice of material for this application. While we are all for improving where we can and optimizing devices and processes to reduce their impact, we feel that this misses the point, the bigger picture. Our desire as future engineers is to be critical of the whole process, the whole application, or even the whole sector we are working on. While this might of course not always be within our reach, it is in our power to choose how to invest our energy and our time. We hope that this thought is shared by many, and that the engineering world will evolve to be more critical of its practices, to dare putting an end to projects that bring more harm than good, to accept not pursuing dreams that are selfish in this context.

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Appendix A

Resonator Design Layout

A.1 Drawing

Figure A.1 shows all design variations of the resonators used in this work. Aside from the top part, this is the exact layout of one die of resonators. The mask contains many repetitions of this die. The top part, with rotated resonators, is in fact part of another type of die, which is present on selected areas of the mask. Rotated resonators also exist in non-rotated form in the main die, where they are identified by alphabet letters.

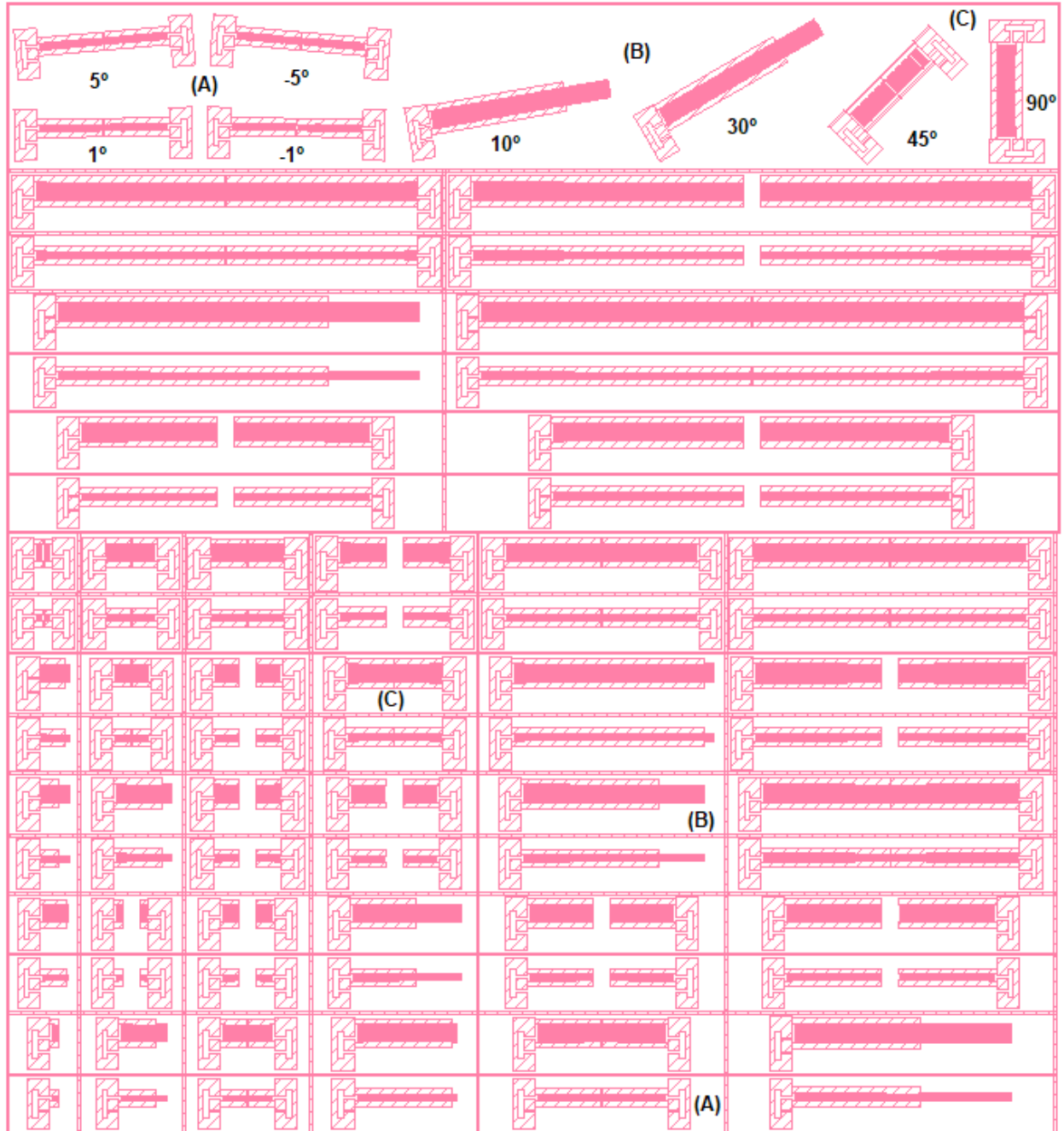


Figure A.1: Designs of resonators present on one die

A.2 Specifications

Figure A.3 compiles the specifications for all variations of resonators. Those specifications are synthesized on Figure A.2 in order to facilitate the interpretation of the notation used in the layout table.

Wavelength (μm) _ Aperture width (μm)
 Number of IDT fingers _ Number of mirror fingers
 Port spacing (μm) *only for devices with two ports*

Figure A.2: Legend of the specifications nomenclature

16_150 100_10 16		16_150 100_100 160	
16_50 100_10 16		16_50 100_100 160	
16_150 100_100		16_150 100_100 16	
16_50 100_100		16_50 100_100 16	
8_150 100_100 160		16_150 100_10 160	
8_50 100_100 160		16_50 100_10 160	
2_150 20_10 16	8_150 20_10 16	2_150 100_100 16	16_150 20_10 160
2_50 20_10 16	8_50 20_10 16	2_50 100_100 16	16_50 20_10 160
8_150 20_10	2_150 20_100 16	2_150 100_10 160	16_150 20_10 16
8_50 20_10	2_50 20_100 16	2_50 100_10 160	16_50 20_10 16
2_150 20_100	16_150 20_10	8_150 20_10 160	2_150 100_100 160
2_50 20_100	16_50 20_10	8_50 20_10 160	2_50 100_100 160
2_150 100_10	2_150 20_10 160	2_150 20_100 160	8_150 20_100 160
2_50 100_10	2_50 20_10 160	2_50 20_100 160	8_50 20_100 160
2_150 20_10	2_150 100_100	2_150 100_10 16	8_150 100_10
2_50 20_10	2_50 100_100	2_50 100_10 16	8_50 20_100

Figure A.3: Specifications of resonators present on one die

A.3 Dimensions

Figure A.4 lists the dimensions of all the resonators. The layout has been automatically defined so that the total surface used by the die is minimal. The dimensions of the whole die are 9371 μm x 8600 μm . All dimensions are in μm , which means that the area of the die is a bit smaller than a cm^2 .

3900X554				5484X554	
3900X520				5484X520	
3900X554				5484X554	
3900X520				5484X520	
3900X554				5484X554	
3900X520				5484X520	
637X554	938X554	1137X554	1484X554	2218X554	2938X554
637X520	938X520	1137X520	1484X520	2218X520	2938X520
637X554	938X554	1137X554	1484X554	2218X554	2938X554
637X520	938X520	1137X520	1484X520	2218X520	2938X520
637X554	938X554	1137X554	1484X554	2218X554	2938X554
637X520	938X520	1137X520	1484X520	2218X520	2938X520
637X542	938X542	1137X542	1484X542	2218X542	2938X542
637X520	938X520	1137X520	1484X520	2218X520	2938X520
637X554	938X554	1137X554	1484X554	2218X554	2938X554
637X520	938X520	1137X520	1484X520	2218X520	2938X520

Figure A.4: Dimensions of resonators present on one die

A.4 Main resonators used in this work

This section presents some resonators that are part of the 72 located on the die, and that were used in our work. Some of them are used mainly because they are the ones which are available in rotated form in the mask. Those resonators are identified by letters A,B and C on the layout (Figure A.1). Others, numbered from 1 to 4, have been used as basis for the geometry study and the technology comparison. Contact pads and busbars of all resonators have the same dimensions.

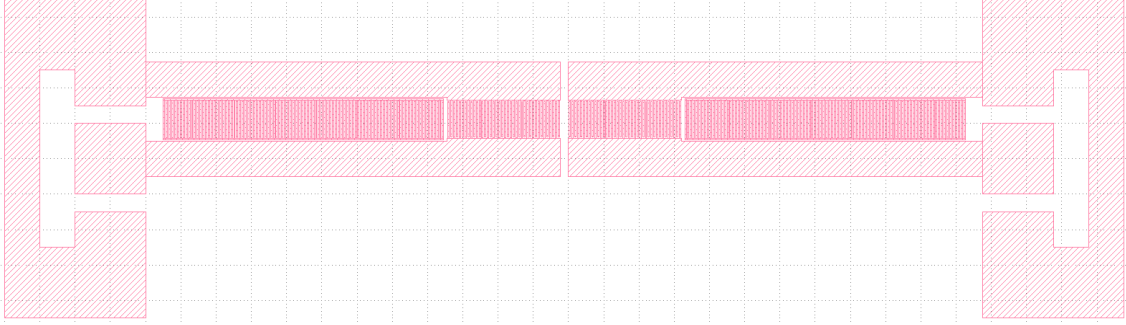


Figure A.5: Resonator A : 2-port, 8 μm wavelength, 50 μm aperture width, 20 IDT fingers, 100 mirror fingers, 16 μm port spacing

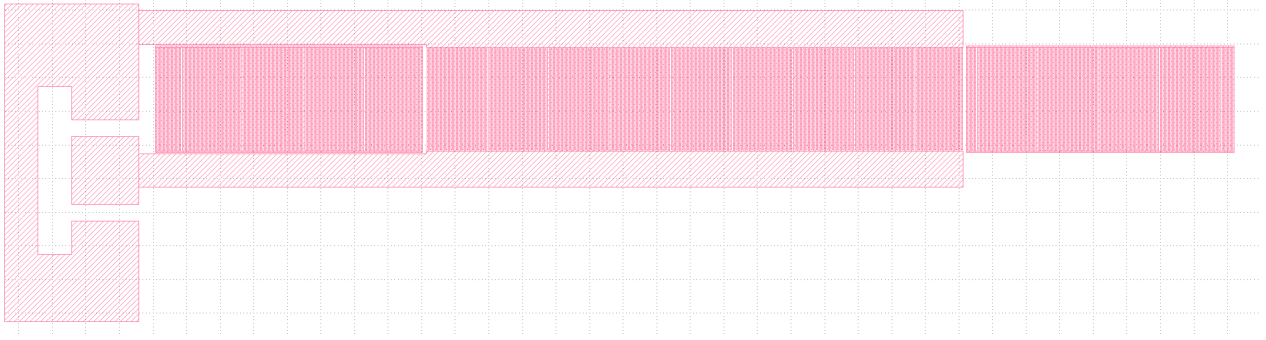


Figure A.6: Resonator B : 1-port, 8 μm wavelength, 150 μm aperture width, 100 IDT fingers, 100 mirror fingers

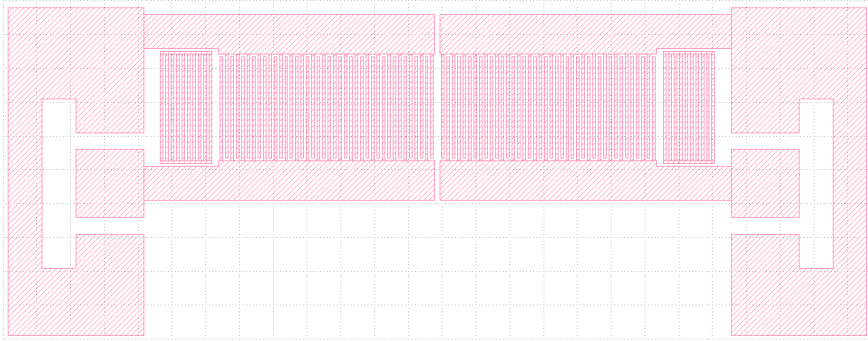


Figure A.7: Resonator C : 2-port, 16 μm wavelength, 150 μm aperture width, 20 IDT fingers, 10 mirror fingers, 16 μm port spacing

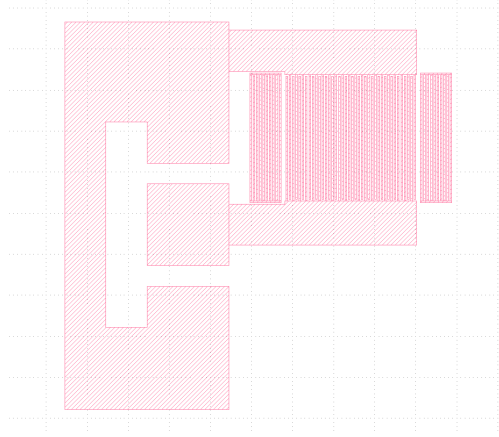


Figure A.8: Resonator 1 : 1-port, 8 μm wavelength, 150 μm aperture width, 20 IDT fingers, 10 mirror fingers

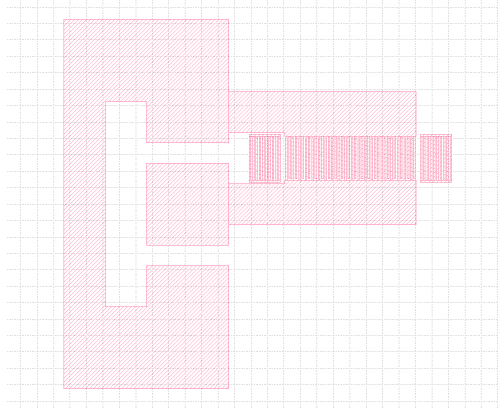


Figure A.9: Resonator 1 : 1-port, 8 μm wavelength, 50 μm aperture width, 20 IDT fingers, 10 mirror fingers

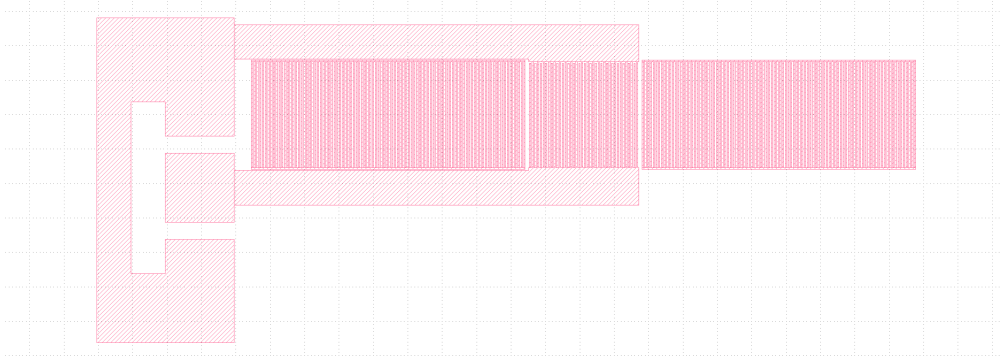


Figure A.10: Resonator 1 : 1-port, 8 μm wavelength, 150 μm aperture width, 20 IDT fingers, 100 mirror fingers

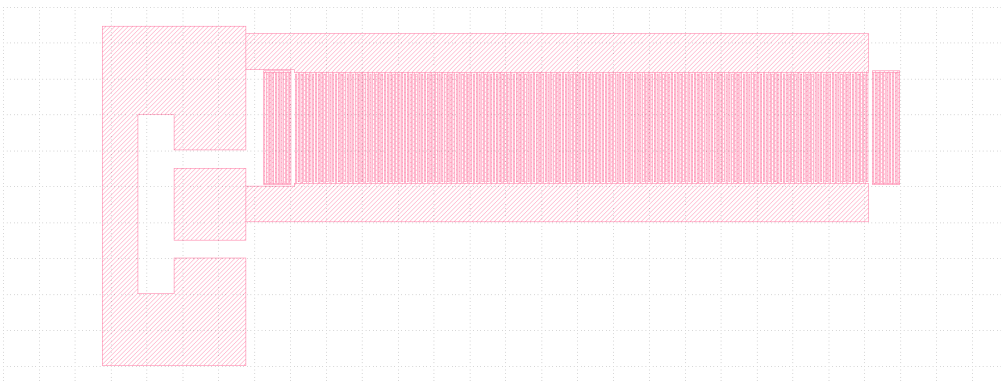


Figure A.11: Resonator 1 : 1-port, 8 μm wavelength, 150 μm aperture width, 100 IDT fingers, 10 mirror fingers

Appendix B

Fabrication steps detail

This section thoroughly explains all iterations of our fabrication process, including failures and improvements, with the aim of guiding any other researcher conducting similar experiments.

B.1 Bulk wafer 1

The first wafer we had at our disposal was actually directly provided by Incize with the resonators fabricated on it. Nevertheless, the process has been described to us and is outlined here.

1. Cleaning : cleaning process of acetone and isopropanol (or methanol), then rinsing with water and drying with nitrogen.
2. Photoresist coating : photoresist was spin-coated in the Süß Gamma 80. nLOF 5510 resin was spin-coated at 1800 rpm.
3. Pre-exposure bake : this step evaporates the solvents present in the resin. The wafer was baked at 90°C for 60 seconds in the Süß Gamma 80 oven.
4. Photolithography : the lithography was performed in the Süß MA6. Vacuum contact with the mask was used. Different exposure doses were tried by hiding some parts of the wafer. 110, 120, 125, 130, 140 and 150 mJ/cm^2 were used.
5. Post-exposure bake : after the photolithography, the wafer is baked again in the Süß Gamma 80 oven. Parameters were not available for this process step.
6. Development : 2 *cl* of developer (AZ 726 MIF) are poured on the wafer. After 60 seconds, the wafer is abundantly rinsed during at least another minute, then dried.
7. Metallization : a 400 nm thickness Al layer was then deposited by evaporation in the VST-TFDS 462.
8. Lift-off : lift-off was performed in an acetone bath, and enhanced with ultrasounds at 80 kHz during 40 minutes.

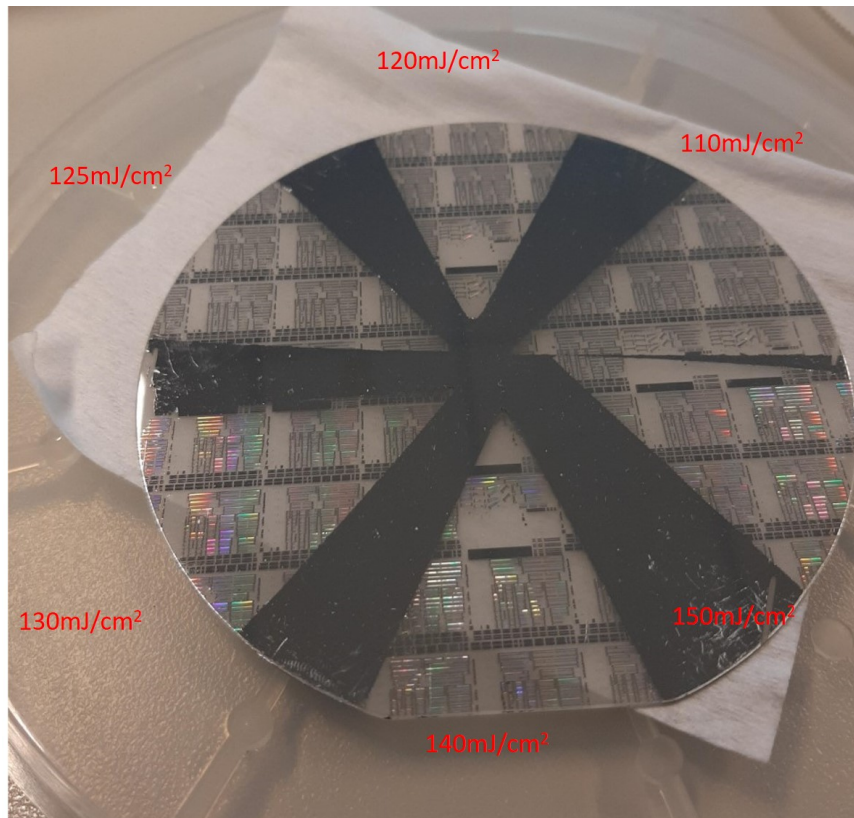


Figure B.1: Wafer "1"

B.2 Bulk wafer 2

The second bulk LiTaO_3 wafer processed has in fact been processed twice, as it broke during the first process. As it broke in large pieces, one of those pieces was used to test plasma etching as an alternative to lift-off

B.2.1 Failure in the midst of the process

Here are the steps that were undertaken before failure.

1. Cleaning : cleaning process of acetone and isopropanol (or methanol), then rinsing with water and drying with nitrogen.
2. Adhesion promotion : this was performed in an LP-III vacuum oven. In the oven, the water contained in the wafer is evaporated by a series of heated (120°C) evacuations and N_2 refills. Then hexamethyldisilazane (HMDS) flows into the evacuated chamber, forming a monolayer on the surface of the wafer that enhances the adhesion of the photoresist. This process is called HMDS vapor priming and takes about 20 minutes.
3. Photoresist coating : nLOF 5510 photoresist was spin-coated in the Süß Gamma 80.
4. Pre-exposure bake : this step evaporates the solvents present in the resin. The wafer was baked in the Süß Gamma 80 oven. Parameters are unavailable for this process step.
5. Photolithography : the lithography was performed in the Süß MA6. Vacuum contact with the mask was used.

Failure occurred during this last photolithography step. Our hypothesis is that it was already fragilized by pyroelectric arcs. Indeed, when taking the wafer out of the LP-III oven (for the adhesion promotion step), we observed a small crack on its surface. We suppose that this crack propagated during the vacuum contact process of the photolithography. This is how we discovered the impact of pyroelectricity, and later took a series of precautions to avoid it.

B.2.2 Plasma etching

We decided to test plasma etching as an alternative to lift-off on the piece of broken wafer, as it was suggested to us to try and compare the resolution with that obtained by lift-off. The process steps are outlined below. This process is also the first one with precautions taken with regard to pyroelectricity.

1. Cleaning : cleaning process of acetone and isopropanol (or methanol), then rinsing with water and drying with nitrogen.
2. Metallization : a 200 nm thickness Al layer was then deposited by evaporation in the VST-TFDS 462.
3. Heating : the wafer was then heated on a heating plate to evaporate the water that had been adsorbed by the aluminium layer. In order to avoid any pyroelectric effect, the wafer was heated incrementally, from room temperature to 110°C, with increments of 10°C every minute.
4. Photoresist coating : AZMIR 701 photoresist was spin-coated at 4000 rpm in the Süß Gamma 80.
5. Pre-exposure bake : this step evaporates the solvents present in the resin. The wafer was baked at 90°C for 90 seconds in the Süß Gamma 80 oven. Precaution is also taken here with regards to pyroelectricity : the oven has pins to hold the wafer in the oven, which then slide down to initiate contact between the wafer and the heating plate of the oven. To ensure gradual heating, the pins are maintained in the top position for a few minutes when the wafer is placed, before being put down.
6. Photolithography : the lithography was performed in the Süß MA6. Vacuum contact with the mask was used. Different exposure doses were tried by hiding some parts of the wafer. 150 and 180 mJ/cm^2 were used.
7. Post-exposure bake : after the photolithography, the wafer is baked again in the Süß Gamma 80 oven, this time at 110°C for 90 seconds. Again, a precautionary wait of a few minutes is observed when the wafer is placed on the pins, before allowing it to touch the heating part.
8. Development : 2 *cl* of developer (AZ 726 MIF) are poured on the wafer. After 60 seconds, the wafer is abundantly rinsed during at least another minute, then dried.
9. Plasma etching : we used a chlorine based process, with gases BCl_3 (5 cm^3/min) and Cl_2 (25 cm^3/min). CH_3 was also used to stop the etching. Other parameters were : ICP (inductively coupled plasma) 300 W, RF 100 W, RF bias -1.2 V. The etching was performed for 20 seconds in the Corial 210 IL ¹.
10. Cleaning : cleaning process to remove the remaining photoresist, with acetone and isopropanol (or methanol), then rinsing with water and drying with nitrogen.

¹Winfab page : https://sites.uclouvain.be/winfab/NEW_website/Public/Facilities/Etching.php - ICP RIE etching part

Manufacturer page : <https://corial.plasmatherm.com/en/products/corial-210il-icp-rie-etch-tool>

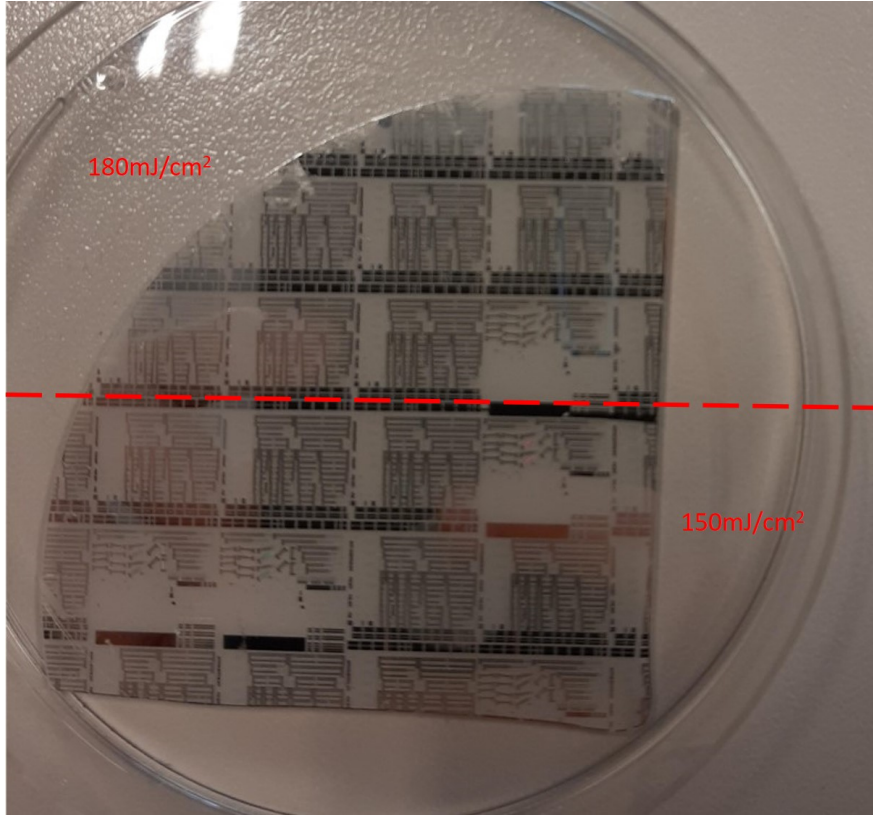


Figure B.2: Wafer "2" realised with plasma etching

B.3 Bulk wafer 3

As plasma etching did not seem better than lift-off in terms of resolution, we decided to stick with the lift-off process. Another wafer was produced with lift-off, taking additional precautions for pyroelectricity. We introduced cooling steps for the wafer to cool down in the air under laminar flow after heating steps such as baking or water evaporation steps.

1. Cleaning : cleaning process of acetone and isopropanol (or methanol), then rinsing with water and drying with nitrogen.
2. Heating : in order to avoid any pyroelectric effect, the wafer is progressively heated on a heating plate, from room temperature to 110°C , with increments of approximately $10^{\circ}/\text{min}$.
3. Adhesion promotion : this was performed in an LP-III vacuum oven. In the oven, the water contained in the wafer is evaporated by a series of heated (120°C) evacuations and N_2 refills. Then hexamethyldisilazane (HMDS) flows into the evacuated chamber, forming a monolayer on the surface of the wafer that enhances the adhesion of the photoresist. This process is called HMDS vapor priming and takes about 20 minutes.
4. Cooling down : this is another step to avoid manifestations of pyroelectricity. Indeed, contact with the cold (room temperature) coating plate might induce a significant temperature gradient. The wafer is simply held in the air under laminar flow (to avoid unwanted particle deposition) until it reaches room temperature.
5. Photoresist coating : photoresist was spin-coated in the Süß Gamma 80. nLOF 5510 resin was spun at 3000 rpm.
6. Pre-exposure bake : this step evaporates the solvents present in the resin. The wafer was baked at 95°C for 90 seconds in the Süß Gamma 80 oven. Precaution is also taken here with regards to pyroelectricity : the oven has pins to hold the wafer in the oven, which then slide down

to initiate contact between the wafer and the heating plate of the oven. To ensure gradual heating, the pins are maintained in the top position for a few minutes when the wafer is placed, before being put down.

7. Photolithography : the lithography was performed in the Süss MA6. Vacuum contact with the mask was used. Different exposure doses were tried by hiding some parts of the wafer. 80, 100, 125, 140, 155 and 180 mJ/cm^2 were used, with doses up until 100 giving acceptable results, with the smaller doses giving the best output.
8. Post-exposure bake : after the photolithography, the wafer is baked again in the Süss Gamma 80 oven, this time at 110°C for 70 seconds. Again, a precautionary wait of a few minutes is observed when the wafer is placed on the pins, before allowing it to touch the heating part.
9. Cooling down : another step to avoid pyroelectricity. Indeed, contact with the cold (room temperature) development plate might induce a significant temperature gradient. The wafer is simply held in the air under laminar flow (to avoid unwanted particle deposition) until it reaches room temperature.
10. Development : 2 *cl* of developer (AZ 726 MIF) are poured on the wafer. After 60 seconds, the wafer is abundantly rinsed during at least another minute, then dried.
11. Metallization : a 200 nm thickness Al layer was then deposited by evaporation in the VST-TFDS 462.
12. Lift-off : lift-off was performed in an acetone bath, and enhanced with ultrasounds at 80 kHz.

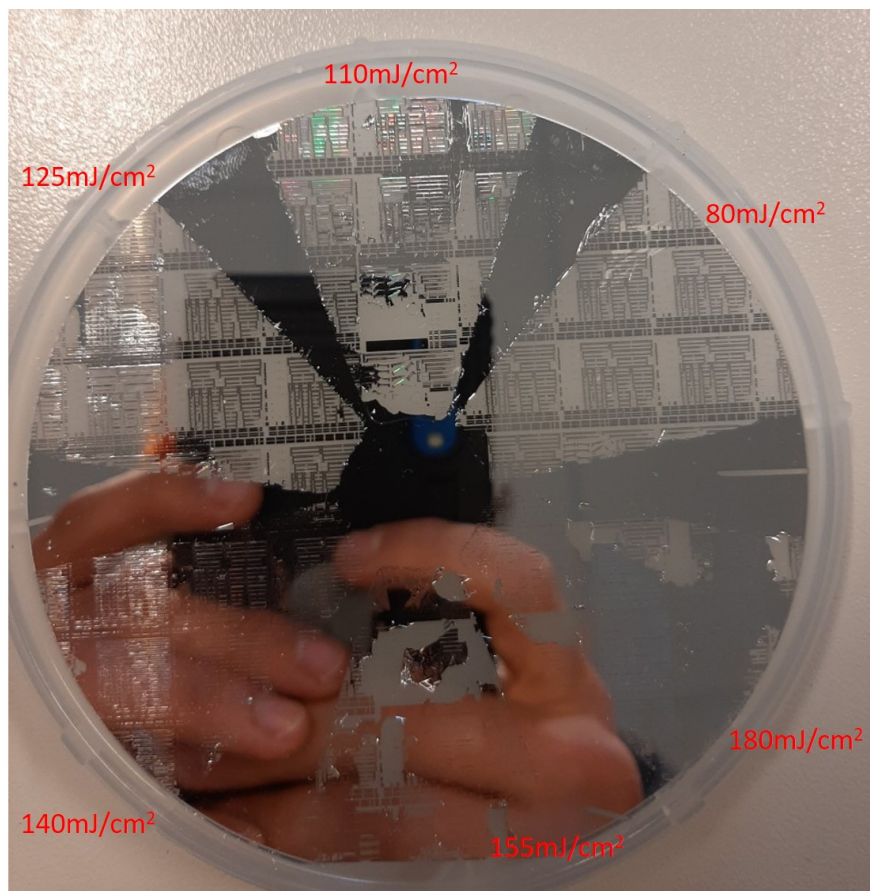


Figure B.3: Wafer "3"

B.3.1 Bulk wafer 4

Finally, as the quality of the lift-off was still not satisfactory, we used another resin, the nLOF 2020, which is thicker and has better adhesion. The choice of resin is often a trade-off as the thicker nLOF 2020 has a worse resolution than the thinner nLOF5510. Regardless, the decision was facilitated by the fact that the smallest resonators (those of 2 μm wavelength) were in all cases not correctly fabricated, as their characteristic dimension of 500 nm (both the width of the electrode fingers and the pitch between them) is around the limit for lift-off and plasma etching processes.

1. Cleaning : the first mandatory step when handling wafers is to clean them to ensure no unwanted particles are present on its surface. Here, the lithium tantalate wafers were cleaned using a rather "soft" cleaning process of acetone and isopropanol (or methanol), then rinsing with water and drying with nitrogen. Hydrofluoric acid HF was avoided as we did not want to risk damaging the wafer surface.
2. Heating : in order to avoid any pyroelectric effect, the wafer is progressively heated on a heating plate, from room temperature to 110°C, with increments of approximately 10°/min.
3. Adhesion promotion : this was performed in an LP-III vacuum oven. In the oven, the water contained in the wafer is evaporated by a series of heated (120°C) evacuations and N₂ refills. Then hexamethyldisilazane (HMDS) flows into the evacuated chamber, forming a monolayer on the surface of the wafer that enhances the adhesion of the photoresist. This process is called HMDS vapor priming and takes about 20 minutes.
4. Cooling down : this is another step to avoid manifestations of pyroelectricity. Indeed, contact with the cold (room temperature) coating plate might induce a significant temperature gradient. The wafer is simply held in the air under laminar flow (to avoid unwanted particle deposition) until it reaches room temperature.
5. Photoresist coating : photoresist was spin-coated in the Süß Gamma 80. nLOF2020 resin was spun at 3000 rpm.
6. Pre-exposure bake : this step evaporates the solvents present in the resin. The wafer was baked at 95°C for 90 seconds in the Süß Gamma 80 oven. Precaution is also taken here with regards to pyroelectricity : the oven has pins to hold the wafer in the oven, which then slide down to initiate contact between the wafer and the heating plate of the oven. To ensure gradual heating, the pins are maintained in the top position for a few minutes when the wafer is placed, before being put down.
7. Photolithography : the lithography was performed in the Süß MA6. Vacuum contact with the mask was used. Different exposure doses were tried by hiding some parts of the wafer. 60, 80, 100, 120, 140 and 160 mJ/cm^2 were used, with doses up until 100 giving acceptable results, with the smaller doses giving the best output.
8. Post-exposure bake : after the photolithography, the wafer is baked again in the Süß Gamma 80 oven, this time at 110°C for 90 seconds. Again, a precautionary wait of a few minutes is observed when the wafer is placed on the pins, before allowing it to touch the heating part.
9. Cooling down : another step to avoid pyroelectricity. Indeed, contact with the cold (room temperature) development plate might induce a significant temperature gradient. The wafer is simply held in the air under laminar flow (to avoid unwanted particle deposition) until it reaches room temperature.
10. Development : 2 *cl* of developer (AZ 726 MIF) are poured on the wafer. After 60 seconds, the wafer is abundantly rinsed during at least another minute, then dried.
11. Metallization : a 200 nm thickness Al layer was then deposited by evaporation in the VST-TFDS 462.

12. Lift-off : lift-off was performed in an acetone bath, and enhanced with ultrasounds at 80 kHz.

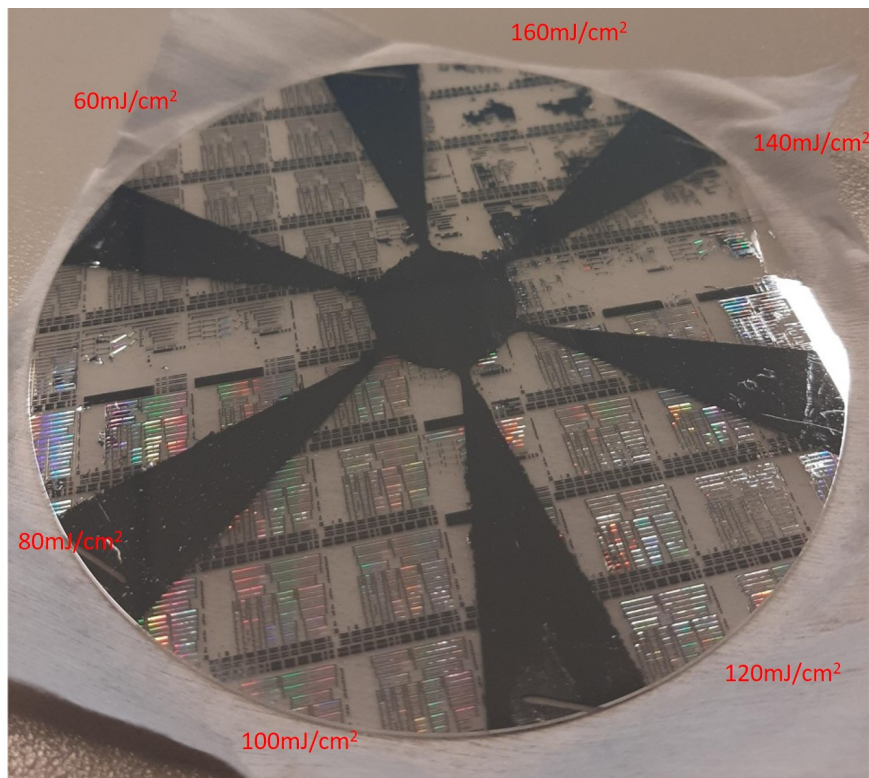


Figure B.4: Wafer "4"

B.3.2 POI wafer

For the fabrication of the POI wafer, we used the exact same parameters as the last bulk wafer. This was intended as a starting point that we could tweak with further experiments, but it proved satisfactory.

1. Cleaning : the first mandatory step when handling wafers is to clean them to ensure no unwanted particles are present on its surface. Here, the lithium tantalate wafers were cleaned using a rather "soft" cleaning process of acetone and isopropanol (or methanol), then rinsing with water and drying with nitrogen. Hydrofluoric acid HF was avoided as we did not want to risk damaging the wafer surface.
2. Heating : in order to avoid any pyroelectric effect, the wafer is progressively heated on a heating plate, from room temperature to 110°C, with increments of approximately 10°/min.
3. Adhesion promotion : this was performed in an LP-III vacuum oven. In the oven, the water contained in the wafer is evaporated by a series of heated (120°C) evacuations and N₂ refills. Then hexamethyldisilazane (HMDS) flows into the evacuated chamber, forming a monolayer on the surface of the wafer that enhances the adhesion of the photoresist. This process is called HMDS vapor priming and takes about 20 minutes.
4. Cooling down : this is another step to avoid manifestations of pyroelectricity. Indeed, contact with the cold (room temperature) coating plate might induce a significant temperature gradient. The wafer is simply held in the air under laminar flow (to avoid unwanted particle deposition) until it reaches room temperature.
5. Photoresist coating : photoresist was spin-coated in the Süß Gamma 80. XXX resin was spinned at 3000 rpm.

6. Pre-exposure bake : this step evaporates the solvents present in the resin. The wafer was baked at 90°C for 90 seconds in the Süß Gamma 80 oven. Precaution is also taken here with regards to pyroelectricity : the oven has pins to hold the wafer in the oven, which then slide down to initiate contact between the wafer and the heating plate of the oven. To ensure gradual heating, the pins are maintained in the top position for a few minutes when the wafer is placed, before being put down. The photoresist layer has been measured to be 1.9 μm thick.
7. Photolithography : the lithography was performed in the Süß MA6. Vacuum contact with the mask was used. Different exposure doses were tried by hiding some parts of the wafer. 60, 80, 100, 120, 140 and 160 mJ/cm^2 were used, with doses up until 100 giving acceptable results, with the smaller doses giving the best output.
8. Post-exposure bake : after the photolithography, the wafer is baked again in the Süß Gamma 80 oven, this time at 110°C for 90 seconds. Again, a precautionary wait of a few minutes is observed when the wafer is placed on the pins, before allowing it to touch the heating part.
9. Cooling down : another step to avoid pyroelectricity. Indeed, contact with the cold (room temperature) development plate might induce a significant temperature gradient. The wafer is simply held in the air under laminar flow (to avoid unwanted particle deposition) until it reaches room temperature.
10. Development : 2 *cl* of developer (AZ 726 MIF) are poured on the wafer. After 60 seconds, the wafer is abundantly rinsed during at least another minute, then dried.
11. Metallization : a 200 nm thickness Al layer was then deposited by evaporation in the VST-TFDS 462.
12. Lift-off : lift-off was performed in an acetone bath, and enhanced with ultrasounds at 80 kHz.

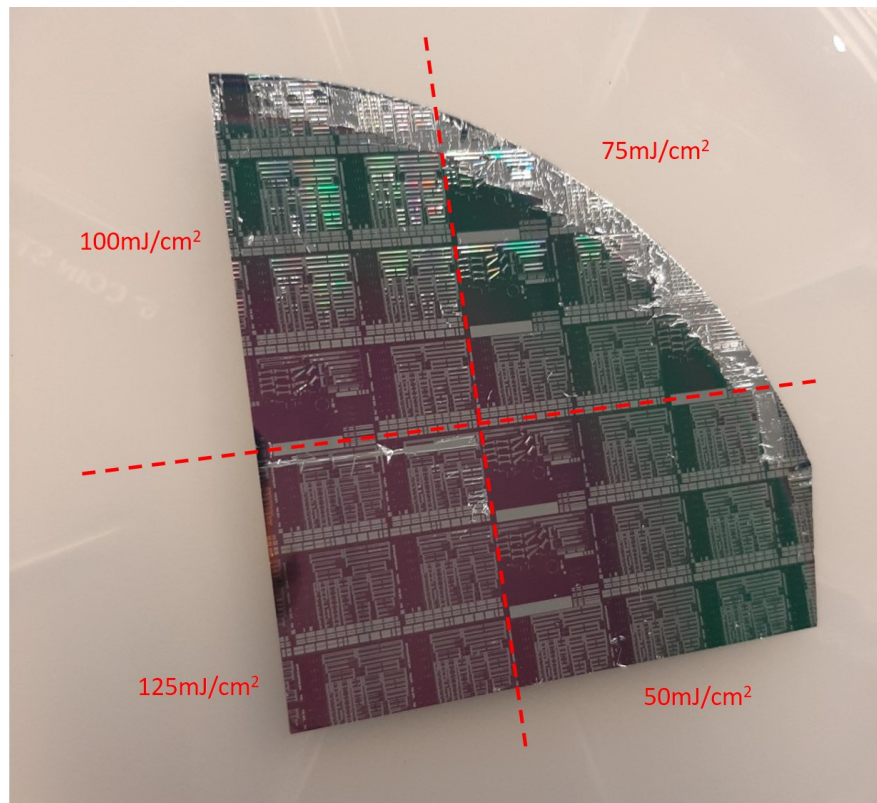


Figure B.5: POI wafer

Appendix C

Computation of resonance and antiresonance frequency

The origin of resonance and antiresonance frequencies in resonators can be easily explained with the simple BVD model only composed of L_m and C_m in the motional branch and C_0 in the static branch, as shown in Figure C.1. The resonance frequency, also called the series frequency, comes

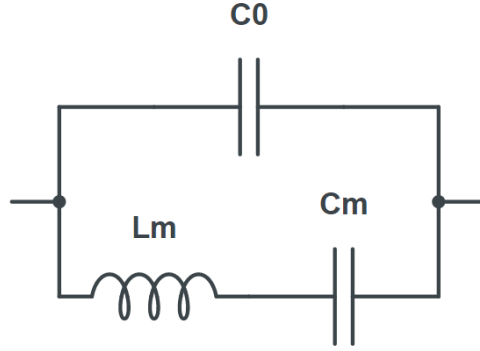


Figure C.1: Simplest BVD model, equivalent circuit for piezoelectric resonator

from the series resonance between L_m and C_m which gives a zero impedance at a certain frequency. Indeed, the impedance of the motional branch (Z_m) is shown at equation (C.1).

$$\begin{aligned} Z_m &= j\omega L_m + \frac{1}{j\omega C_m} \\ &= j\left(\omega L_m - \frac{1}{\omega C_m}\right) \\ &= j\left(\frac{\omega^2 L_m C_m - 1}{\omega C_m}\right) \end{aligned} \tag{C.1}$$

This impedance can be equalized to zero at the resonance frequency f_r .

$$\begin{aligned} (2\pi f_r)^2 L_m C_m - 1 &= 0 \\ f_r &= \frac{1}{2\pi} \sqrt{\frac{1}{L_m C_m}} \end{aligned} \tag{C.2}$$

For this frequency, the impedance of the motional branch is equal to zero.

The antiresonance phenomenon is caused by the parallel resonance between both branches and results in an infinite impedance. The impedance of both branches in parallel (Z_p) is developed at

equation C.3.

$$\begin{aligned}
Z_p &= (\frac{-j\omega C_m}{\omega^2 L_m C_m - 1} + j\omega C_0)^{-1} \\
&= j(\frac{\omega C_m - \omega^3 L_m C_m C_0 + \omega C_0}{\omega^2 L_m C_m - 1})^{-1} \\
&= j(\frac{\omega^2 L_m C_m - 1}{\omega(C_m + C_0 - \omega^2 L_m C_m C_0)})
\end{aligned} \tag{C.3}$$

The resonance between L_m and C_m is present at the numerator and it is clear that the resonance will cause a zero impedance in the parallel circuit too. Furthermore, the impedance will be infinite when the denominator will be equal to zero, at the antiresonance frequency f_a .

$$\begin{aligned}
C_m + C_0 - (2\pi f_a)^2 L_m C_m C_0 &= 0 \\
(2\pi f_a)^2 &= \frac{C_m + C_0}{L_m C_m C_0} \\
f_a &= \frac{1}{2\pi} \sqrt{\frac{C_m + C_0}{L_m C_m C_0}}
\end{aligned} \tag{C.4}$$

At this frequency, the impedance of the equivalent circuit is infinite, we thus have the antiresonance.

Appendix D

Materials properties on COMSOL

D.1 Aluminium

Property	Variable	Value	Unit	Property group
Relative permittivity	epsilon _{nr_iso} ; epsilon _{nrii} = epsilon _{nr_iso} , epsilon _{nrij} = 0	1	1	Basic
Density	rho	2700	kg/m ³	Basic
Young's modulus	E	70e9	Pa	Young's modulus and Poisson's ratio
Poisson's ratio	nu	0.33	1	Young's modulus and Poisson's ratio
Relative permeability	mu _{r_iso} ; mu _{rii} = mu _{r_iso} , mu _{r_{ij}} = 0	1	1	Basic
Heat capacity at constant pressure	C _p	900	J/(kg·K)	Basic
Thermal conductivity	k _{iso} ; k _{ii} = k _{iso} , k _{ij} = 0	238	W/(m·K)	Basic
Electrical conductivity	sigma _{iso} ; sigma _{aii} = sigma _{iso} , sigma _{aij} = 0	3.774e7	S/m	Basic
Coefficient of thermal expansion	alpha _{iso} ; alpha _{aii} = alpha _{iso} , alpha _{aij} = 0	23e-6	1/K	Basic
Murnaghan third-order elastic moduli	l	-2.5e11	N/m ²	Murnaghan
Murnaghan third-order elastic moduli	m	-3.3e11	N/m ²	Murnaghan
Murnaghan third-order elastic moduli	n	-3.5e11	N/m ²	Murnaghan
Lamé parameter λ	lambLame	5.1e10	N/m ²	Lamé parameters
Lamé parameter μ	muLame	2.6e10	N/m ²	Lamé parameters

D.2 Silicon oxide

Property	Variable	Value	Unit	Property group
Relative permittivity	ϵ_{nr_iso} ; $\epsilon_{nrii} = \epsilon_{nr_iso}$, $\epsilon_{nrij} = 0$	4.2	1	Basic
Density	ρ	2200	kg/m ³	Basic
Young's modulus	E	70e9	Pa	Young's modulus and Poisson's ratio
Poisson's ratio	ν	0.17	1	Young's modulus and Poisson's ratio
Electrical conductivity	σ_{iso} ; $\sigma_{iia} = \sigma_{iso}$, $\sigma_{iaj} = 0$	0	S/m	Basic
Coefficient of thermal expansion	α_{iso} ; $\alpha_{iia} = \alpha_{iso}$, $\alpha_{iaj} = 0$	0.5e-6	1/K	Basic
Heat capacity at constant pressure	C_p	730	J/(kg·K)	Basic
Thermal conductivity	k_{iso} ; $k_{ii} = k_{iso}$, $k_{ij} = 0$	1.4	W/(m·K)	Basic

D.3 Lithium tantalate

Property	Variable	Value	Unit	Property group
Density	rho	7450	kg/m ³	Basic
Compliance matrix, Voigt notation	{sE11, sE12, sE22, sE13, sE23, sE33, sE14, sE24, sE34, sE44, sE15, sE25, sE35, sE45, sE55, sE16, sE26, sE36, sE46, sE56, sE66} ; sEij = sEji	{4.87e-012, -5.8e-013, 4.87e-012, -1.25e-012, -1.25e-012, 4.36e-012, 6.4e-013, -6.4e-013, 0, 1.08e-011, 0, 0, 0, 0, 1.08e-011, 0, 0, 0, 0, 1.28e-012, 1.09e-011}	1/Pa	Strain-charge form
Coupling matrix, Voigt notation	{dET11, dET21, dET31, dET12, dET22, dET32, dET13, dET23, dET33, dET14, dET24, dET34, dET15, dET25, dET35, dET16, dET26, dET36}	{0, -7e-012, -2e-012, 0, 7e-012, -2e-012, 0, 0, 8e-012, 0, 2.6e-011, 0, 2.6e-011, 0, 0, -1.4e-011, 0, 0}	C/N	Strain-charge form
Relative permittivity	{epsilon_rT11, epsilon_rT22, epsilon_rT33} ; epsilon_rTij = 0	{51, 51, 45}	1	Strain-charge form
Loss factor for elasticity matrix cE	eta_cE_iso ; eta_cEii = eta_cE_iso, eta_cEij = 0	0	1	Stress-charge form
Loss factor for coupling matrix eES	{eta_eES11, eta_eES21, eta_eES31, eta_eES12, eta_eES22, eta_eES32, eta_eES13, eta_eES23, eta_eES33, eta_eES14, eta_eES24, eta_eES34, eta_eES15, eta_eES25, eta_eES35, eta_eES16, eta_eES26, eta_eES36}	{0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0}	1	Stress-charge form
Loss factor for electrical permittivity S	eta_epsilonS_iso ; eta_epsilonSii = eta_epsilonS_iso, eta_epsilonSij = 0	0.007	1	Stress-charge form
Relative permittivity	{epsilon_r11, epsilon_r22, epsilon_r33} ; epsilon_rij = 0	{40.9, 40.9, 43.3}	1	Basic
Loss factor for compliance matrix sE	eta_sE_iso ; eta_sEii = eta_sE_iso, eta_sEij = 0	0	1	Strain-charge form
Loss factor for coupling matrix dET	{eta_dET11, eta_dET21, eta_dET31, eta_dET12, eta_dET22, eta_dET32, eta_dET13, eta_dET23, eta_dET33, eta_dET14, eta_dET24, eta_dET34, eta_dET15, eta_dET25, eta_dET35, eta_dET16, eta_dET26, eta_dET36}	{0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0}	1	Strain-charge form
Loss factor for electrical permittivity T	eta_epsilonT_iso ; eta_epsilonTii = eta_epsilonT_iso, eta_epsilonTij = 0	0.007	1	Strain-charge form
Elasticity matrix, Voigt notation	{cE11, cE12, cE22, cE13, cE23, cE33, cE14, cE24, cE34, cE44, cE15, cE25, cE35, cE45, cE55, cE16, cE26, cE36, cE46, cE56, cE66} ; cEij = cEji	{2.32966e+11, 4.68904e+10, 2.32966e+11, 8.02342e+10, 8.02342e+10, 2.75364e+11, -1.10267e+10, 1.10267e+10, 0, 9.38995e+10, 0, 0, 0, 9.38995e+10, 0, 0, 0, 0, -1.10267e+10, 9.3038e+10}	Pa	Stress-charge form
Coupling matrix, Voigt notation	{eES11, eES21, eES31, eES12, eES22, eES32, eES13, eES23, eES33, eES14, eES24, eES34, eES15, eES25, eES35, eES16, eES26, eES36}	{0, -1.58923, 0.0821598, 0, 1.58923, 0.0821598, 0, 0, 1.88197, 0, 2.59576, 0, 2.59576, 0, 0, -1.58923, 0, 0}	C/m ²	Stress-charge form
Relative permittivity	{epsilon_rS11, epsilon_rS22, epsilon_rS33} ; epsilon_rSij = 0	{40.9, 40.9, 43.3}	1	Stress-charge form

D.4 Polycrystalline silicon

Property	Variable	Value	Unit	Property group
Relative permittivity	epsilon_r_iso ; epsilon_rii = epsilon_r_iso, epsilon_rij = 0	4.5	1	Basic
Density	rho	2320	kg/m ³	Basic
Young's modulus	E	160e9	Pa	Young's modulus and Poisson's ratio
Poisson's ratio	nu	0.22	1	Young's modulus and Poisson's ratio
Coefficient of thermal expansion	alpha_iso ; alpha_ii = alpha_iso, alpha_ij = 0	2.6e-6	1/K	Basic
Heat capacity at constant pressure	Cp	678	J/(kg·K)	Basic
Thermal conductivity	k_iso ; k_ii = k_iso, k_ij = 0	34	W/(m·K)	Basic

D.5 Single-crystal Silicon (substrate)

Property	Variable	Value	Unit	Property group
Relative permittivity	$\epsilon_{\text{r_iso}}$; $\epsilon_{\text{r}ii} = \epsilon_{\text{r_iso}}$, $\epsilon_{\text{r}ij} = 0$	11.7	1	Basic
Density	ρ	2329	kg/m ³	Basic
Young's modulus	E	170e9	Pa	Young's modulus and Poisson's ratio
Poisson's ratio	ν	0.28	1	Young's modulus and Poisson's ratio
Coefficient of thermal expansion	α_{iso} ; $\alpha_{\text{ii}} = \alpha_{\text{iso}}$, $\alpha_{\text{ij}} = 0$	2.6e-6	1/K	Basic
Heat capacity at constant pressure	C_p	700	J/(kg·K)	Basic
Thermal conductivity	k_{iso} ; $k_{\text{ii}} = k_{\text{iso}}$, $k_{\text{ij}} = 0$	130	W/(m·K)	Basic

D.6 Aluminium Nitride

Property	Variable	Value	Unit	Property group
Density	rho	3300	kg/m ³	Basic
Compliance matrix, Voigt notation	{sE11, sE12, sE22, sE13, sE23, sE33, sE14, sE24, sE34, sE44, sE15, sE25, sE35, sE45, sE55, sE16, sE26, sE36, sE46, sE56, sE66} ; sEij = sEji	{2.8987e-12, -9.326e-013, 2.8987e-12, -5.0038e-013, -5.0038e-013, 2.8253e-012, 0, 0, 0, 8E-12, 0, 0, 0, 0, 8E-12, 0, 0, 0, 0, 0, 7.6628E-12}	1/Pa	Strain-charge form
Coupling matrix, Voigt notation	{dET11, dET21, dET31, dET12, dET22, dET32, dET13, dET23, dET33, dET14, dET24, dET34, dET15, dET25, dET35, dET16, dET26, dET36}	{0, 0, -1.9159e-012, 0, 0, -1.9159e-012, 0, 0, 4.9597e-012, 0, -3.84e-012, 0, -3.84e-012, 0, 0, 0, 0, 0}	C/N	Strain-charge form
Relative permittivity	{epsilonIrrT11, epsilonIrrT22, epsilonIrrT33} ; epsilonIrrTij = 0	{9.2081, 9.2081, 10.1192}	1	Strain-charge form
Loss factor for electrical permittivity S	eta_epsilonS_iso ; eta_epsilonSii = eta_epsilonS_iso, eta_epsilonSij = 0	2.1e-3	1	Stress-charge form
Relative permittivity	epsilonIrr_iso ; epsilonIrrii = epsilonIrr_iso, epsilonIrrij = 0	9	1	Basic
Loss factor for compliance matrix sE	eta_sE_iso ; eta_sEii = eta_sE_iso, eta_sEij = 0	0	1	Strain-charge form
Loss factor for coupling matrix dET	{eta_dET11, eta_dET21, eta_dET31, eta_dET12, eta_dET22, eta_dET32, eta_dET13, eta_dET23, eta_dET33, eta_dET14, eta_dET24, eta_dET34, eta_dET15, eta_dET25, eta_dET35, eta_dET16, eta_dET26, eta_dET36}	{0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0}	1	Strain-charge form
Loss factor for electrical permittivity T	eta_epsilonT_iso ; eta_epsilonTii = eta_epsilonT_iso, eta_epsilonTij = 0	0	1	Strain-charge form
Elasticity matrix, Voigt notation	{cE11, cE12, cE22, cE13, cE23, cE33, cE14, cE24, cE34, cE44, cE15, cE25, cE35, cE45, cE55, cE16, cE26, cE36, cE46, cE56, cE66} ; cEij = cEji	{4.1e+011, 1.49e+011, 4.1e+011, 0.99e+011, 0.99e+011, 3.89e+011, 0, 0, 0, 1.25e+011, 0, 0, 0, 0, 1.25e+011, 0, 0, 0, 0, 0, 1.305e+011}	Pa	Stress-charge form
Coupling matrix, Voigt notation	{eES11, eES21, eES31, eES12, eES22, eES32, eES13, eES23, eES33, eES14, eES24, eES34, eES15, eES25, eES35, eES16, eES26, eES36}	{0, 0, -0.58, 0, 0, -0.58, 0, 0, 1.55, 0, -0.48, 0, -0.48, 0, 0, 0, 0, 0}	C/m ²	Stress-charge form
Relative permittivity	epsilonIrrS_iso ; epsilonIrrSii = epsilonIrrS_iso, epsilonIrrSij = 0	9	1	Stress-charge form
Loss factor for elasticity matrix cE	eta_cE_iso ; eta_cEii = eta_cE_iso, eta_cEij = 0	0	1	Stress-charge form
Loss factor for coupling matrix eES	{eta_eES11, eta_eES21, eta_eES31, eta_eES12, eta_eES22, eta_eES32, eta_eES13, eta_eES23, eta_eES33, eta_eES14, eta_eES24, eta_eES34, eta_eES15, eta_eES25, eta_eES35, eta_eES16, eta_eES26, eta_eES36}	{0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0}	1	Stress-charge form

Appendix E

Microscope pictures of resonators

This section shows the resonators with a microscope view.

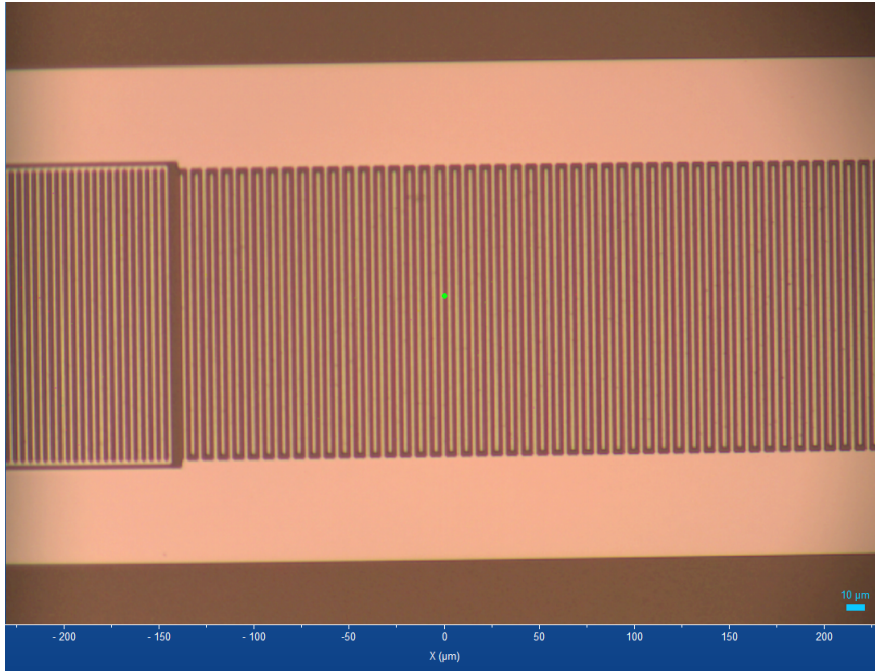


Figure E.1: Resonator B on POI substrate.

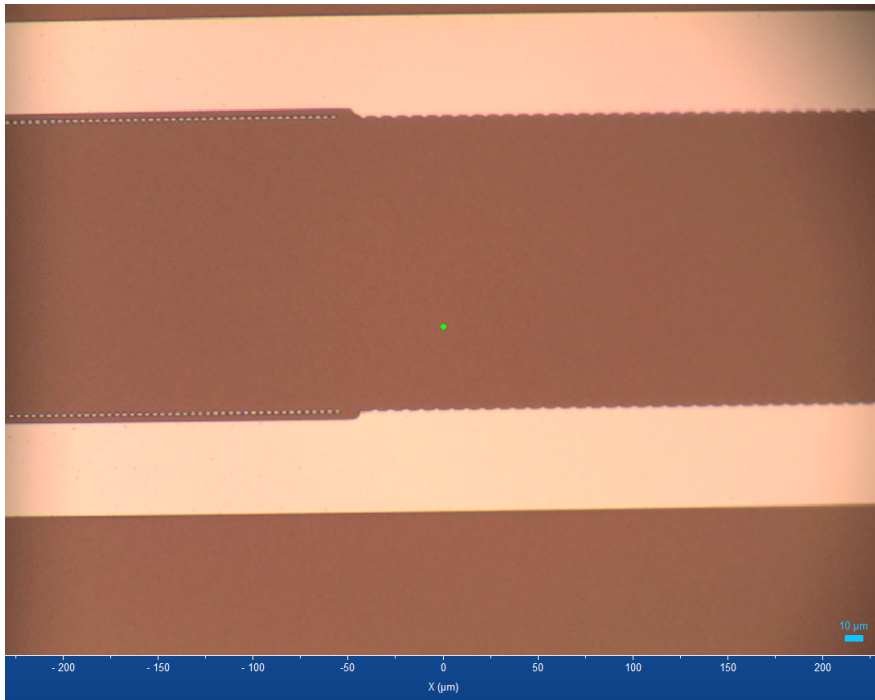


Figure E.2: Resonator B on POI substrate. This resonator is used as an open due to the too high exposure dose ($125\text{mJ}/\text{cm}^2$).

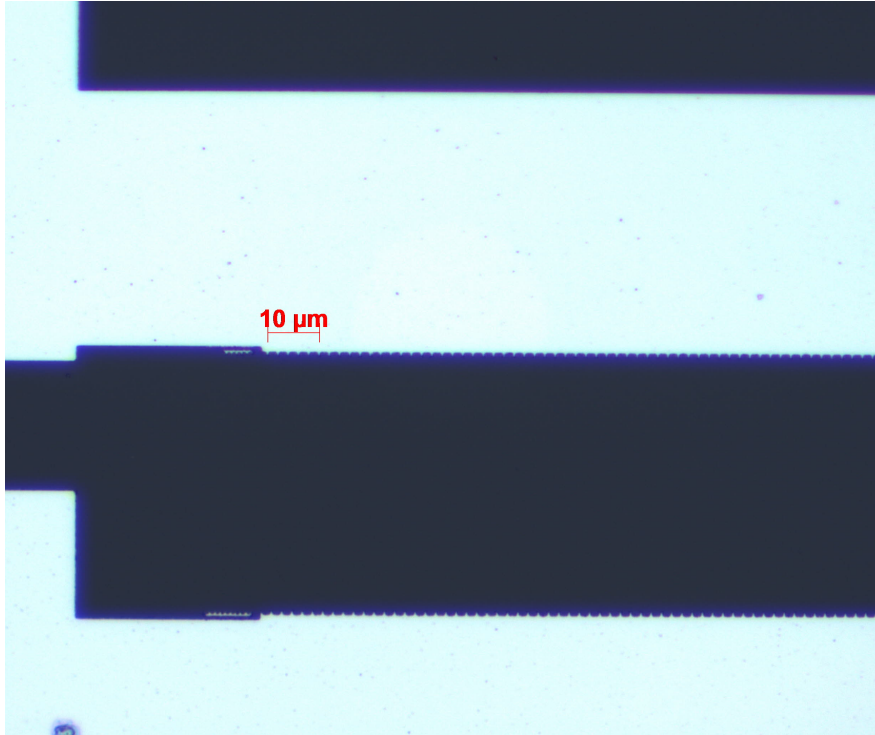


Figure E.3: Resonator of 2 microns wavelength on bulk LT tantalate substrate. This is used as an open due to the too high accuracy which cannot be achieved by the lift of process.

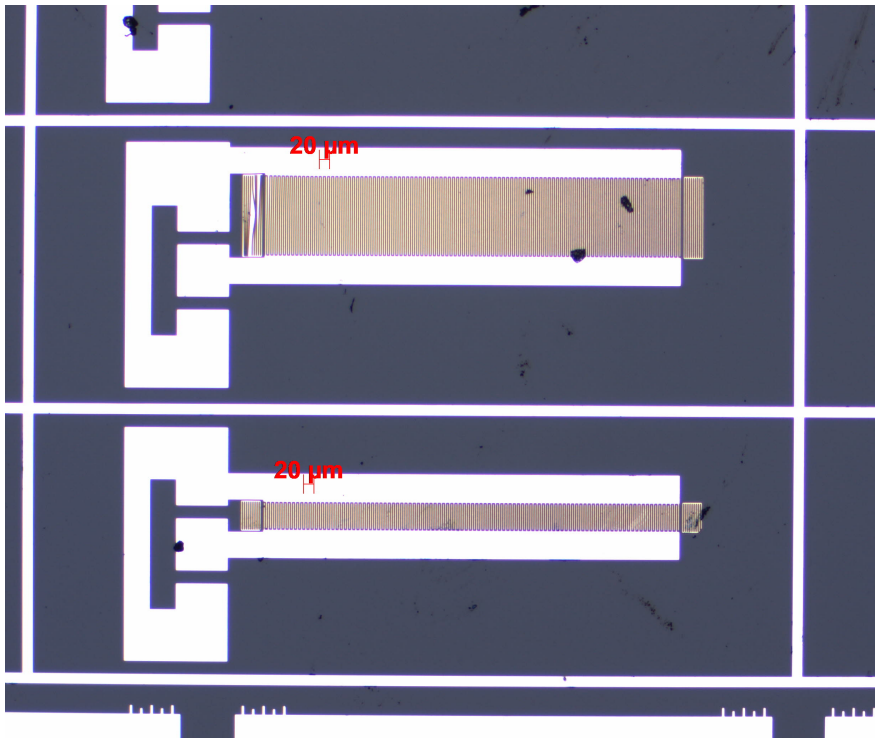


Figure E.4: Part of die with 2 resonators on a bulk LT substrate.

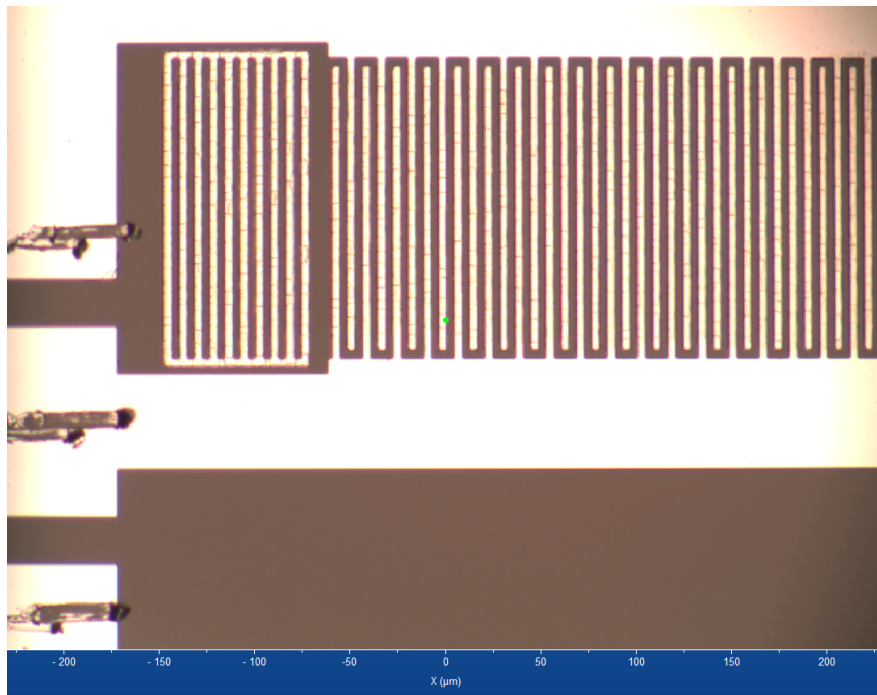


Figure E.5: Resonator on a bulk LT substrate frabricated with plasma etching. The three lignes on the left are traces of the probes in the aluminium.

Appendix F

Extraction of resonator models and comparison

This section presents the way to extract the equivalent models which are presented in section 4.3 (BVD and mBVD) and make a comparison between the method of extraction.

All the parameters and lumped elements could be extracted based on the measurements as explained in section 4.4.5. Unfortunately, the difference of quality factor between resonance and antiresonance, the noise, the inconstant value of R_{stat} , and the fact that this model is based on several different equation makes him quite sensitive. It occurs several time that obtained value where not physically acceptable such that negative resistances. It is thus necessary to have another robust extraction method to compare the different resonators properly.

It does not occurs to the BVD model due to the fact that this model is rather simple.

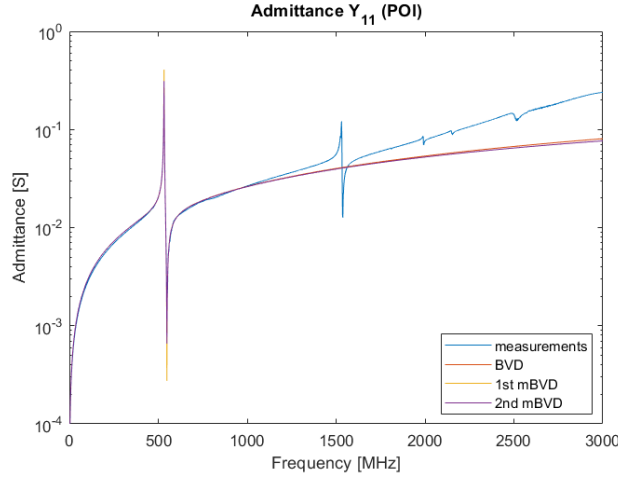
This extraction method is based on the fact that BVD model fit the curve properly close to resonance but is less accurate far from it while mBVD model is closer to the real behaviour everywhere.

Here is thus the method which is done to extract mBVD model. First of all a BVD model is extracted thanks to the measurements close to resonance (except for C_0). Resonance and antiresonance frequencies, and C_0 are extracted as explained in section 4.4.5, R_m is extracted as explained in the BVD part of this section. Then C_m and L_m are computed. Quality factors are also extracted here when the BVD model is chosen.

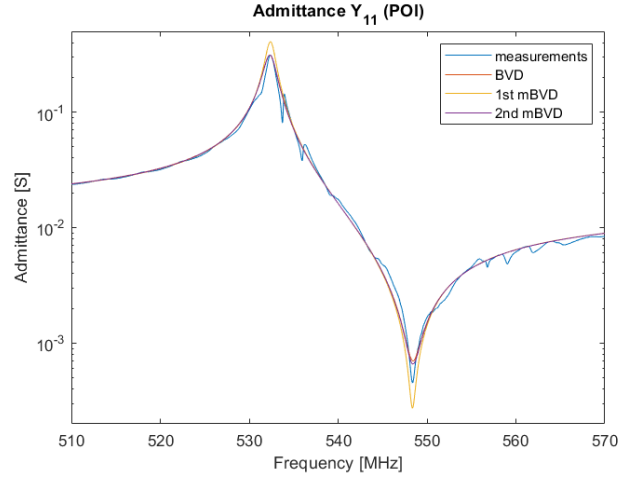
If we want an mBVD model, and once BVD model is complete, the quality factors of the BVD model are computed as explained in section 4.4.5. And R_{stat} is computed on the biggest range of frequency. When f_a , f_r , Q_a , Q_r , C_0 and R_{stat} are known, the complete mBVD model can be found as explained in section 4.4.5.

To compare the different method of extraction and the different model, we use a resonator for which the direct extraction method of mBVD model gives only positive results. The plot of admittance and phase of the admittance are available at figure F.1. The measurements curve is shown, the BVD model directly extracted from the measurements is available too. The curve so-called "1st mBVD" is the mBVD model based on the direct extraction of all its lumped element directly on measurements while "2nd mBVD" corresponds to the model whose extraction is based on the BVD model.

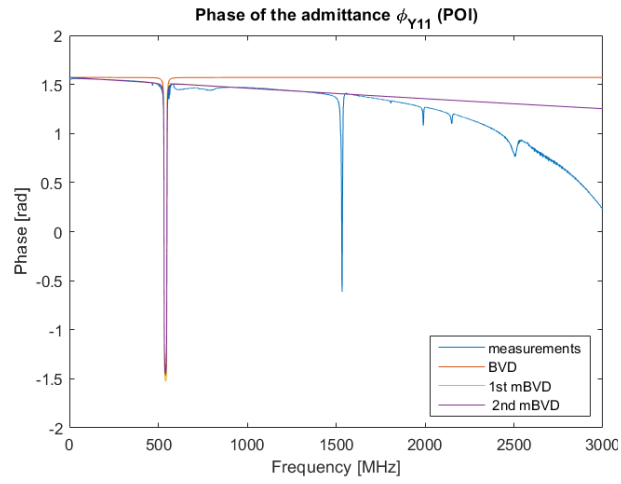
On the admittance plots, we can observe that the BVD and the second mBVD models are quite close, which showcases the validity of the simple BVD model. The wider frequency range of Figure F.1a shows that the models are accurate mainly around the resonance. In the phase plots, we can observe that both mBVD provide better fitting of the measurement data. In particular, the second mBVD model appears to be the best fit. Hence, it is the one we will use to compare bulk LT and POI technologies.



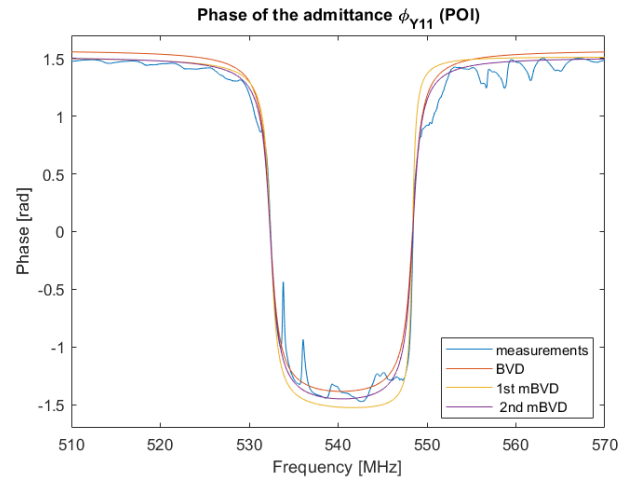
(a) Admittance



(b) Admittance



(c) Phase of the admittance



(d) Phase of the admittance

Figure F.1: Comparison of the different models for POI

Appendix G

Critical Raw material classification

Here, the two indicators used by the EU to determine critical raw materials (section 6.1.2.3) are developed. A raw material is considered critical if EI AND SR overcome a certain threshold, respectively 2.8 and 1.

Economic importance (EI) :

The EI indicates the importance of a material for EU economy. It is computed as follows :

$$EI = \sum_s (A_s * Q_s) * SI_{EI} \quad (G.1)$$

Where :

- EI is the economic importance
- A_s is the share of end use of a raw material in a sector.
- Q_s is the sector's value added.
- SI_{EI} is the substitution index of a raw material related to economic importance.
- s denotes the sector. The different sectors are defined by the NACE Rev. 2 classification [74].

The availability of substitutes reduces the economic importance, this is why there is a substitution index (SI_{EI}). Notice that commercial information and published patents are only used to identify proven substitute alternatives readily available and applicable at the market today. Neither 'substitutability' nor 'potential future substitution' is considered in this methodology [122]. This substitution index is then computed like this :

$$SI_{EI} = \sum_i \sum_a SCP_{i,a} * Share_a * Subshare_{i,a} \quad (G.2)$$

Where :

- i denotes an individual substitute material
- a denotes an individual application of the candidate material (material to be substituted)
- $SCP_{i,a}$ is the substitute cost performance parameter for substitute material i in application a
- $Share_a$ is the share represented by application a in the use of the raw candidate material
- $Subshare_{i,a}$ is the share of candidate material which is substituted by substitute material i , in application a . In other words, it is the share of $Share_a$ substituted by i .

The SCP is there to take into account the fact that the market decision to adopt a substitute material is taken on the basis of its cost and the technical performance and functionality it offers. The different values the SCP can take are describe at figure G.1.

Substitute material technical performance \ Substitute material cost	Similar performance	Reduced performance	Performance in case of no substitute
Very high costs (more than 2 times)	0.9	1	1
Slightly higher costs (up to 2 times)	0.8	0.9	1
Similar or lower costs	0.7	0.8	1

Figure G.1: Possible values of SCP based on the current performance and cost [122]

Supply Risk (SR) :

SR accounts for the risk of disruption in the European supply of a material. It is calculated following equation G.3.

$$SR = \left[(HHI_{WGI,t})_{GS} \cdot \frac{IR}{2} + (HHI_{WGI,t})_{EU_{sourcing}} \left(1 - \frac{IR}{2} \right) \right] \cdot (1 - EoL_{RIR}) \cdot SI_{SR} \quad (G.3)$$

where :

- SR is the supply risk
- $HHI_{WGI,t}$ is the Herfindahl-Hirschman Index, taking into account the World Governance Index WGI and the trade parameter t adjusting WGI . GS denotes global suppliers, while $EU_{sourcing}$ denotes countries that are actual supply sources for the EU
- IR is the import reliance
- EoL_{RIR} is the end-of life recycling input rate
- SI_{SR} is the substitution index related to supply risk

The parameters involved in the calculation of the supply risk SR are further explained below :

- **HHI** : The Herfindahl-Hirschman Index is an indicator of the amount of competition among companies, or in this case countries, within an industry. It ranges from 0 to 1 as a percentage (or sometimes from 0 to 10 000 points), 0 being the case of an infinite number of very small companies/countries, and 1 being the case of a monopoly. It is usually computed as follows:

$$HHI = \sum_{i=1}^n S_i^2 \quad (G.4)$$

where S_i is the market share of company i in the market, and n is the number of companies. Here, $HHI_{WGI,t}$ is used as a proxy for concentration of primary supply from raw materials producing countries. It is computed as :

$$HHI_{WGI,t} = \sum_c S_c^2 * WGI_c * t_c \quad (G.5)$$

where

- S_c is the share of country c within the global supply (or EU sourcing) of the raw material
- WGI_c is the world governance index of country c , used as a proxy for country governance
- t_c is a trade parameter

t_c is used to quantify influence of trade (e.g. trade agreements or export restrictions such as taxes, quotas, prohibitions) on the supply risk related to a specific country c for the supply of the candidate raw material. t_c ranges from 0.8 to 2, and the determination of its value depends on the situation. t_c is either equal to EU_c , $ET - TA_c$, EQ_c or EP_c .

- EU_c : in the case of the supplier country being part of the EU, the risk is considered lowest and therefore $t_c = EU_c = 0.8$.
- $ET - TA_c$: if export taxes (ET) and trade agreements (TA) exist for a non-EU country c , their influence is quantified separately. Export taxes increase the risk and ET takes the following values :
 - * $ET = 1.1$ (if $0 < taxes \leq 25\%$)
 - * $ET = 1.2$ (if $25\% < taxes \leq 75\%$)
 - * $ET = 1.3$ (if $taxes > 75\%$)

The risk mitigating effect of bilateral trade agreements (TA) is assessed on a case-by-case basis.

- EQ_c : Export quotas (EQ) increase the risk associated with country c , for the candidate raw material.

$$EQ_c = 1 + \frac{\text{country } c \text{ production} - \text{physical quota imposed}}{\text{total world production}}$$

- EP_c : Export prohibition (EP) is an extreme case of quota, where the quota is equal to 0.

$$EP_c = 1 + \frac{\text{country } c \text{ production}}{\text{total world production}}$$

- **IR**: The import reliance (IR) is a parameter used to balance the risk linked to the global supply mix and the actual EU sourcing. It is calculated as follow :

$$IR = \frac{\text{Net Import}}{\text{Apparent Consumption}} = \frac{\text{Import} - \text{Export}}{\text{Domestic Production} + \text{Import} - \text{Export}} \quad (\text{G.6})$$

- **EoLRIR**: is a coefficient which aims to reduce the SR if the candidate material is recycled. It is computed that way :

$$EoLRIR = \frac{\text{Input of secondary material}}{\text{Input of secondary material} + \text{Input of primary material}} \quad (\text{G.7})$$

Secondary materials are recycled materials which are used one more time in a manufacturing process. They are opposite to primary materials or virgin materials which are used for the first time in the manufacturing process.

- **SI_{SR}** : As for the EI , a substitution index (SI_{SR}) is added to take into account the substitutes materials. The computation of SI_{SR} is below :

$$SI_{SR} = \sum_i [(SP_i * SCr_i * SCo_i)^{1/3} * \sum_a (Subshare_{i,a} * Share_a)] \quad (\text{G.8})$$

Where :

- i denotes an individual substitute material
- a denotes an individual application of the candidate material (material to be substituted)
- SP_i is the substitute production
- SCr_i is the substitute criticality
- SCo_i is the substitute co-production
- $Share_a$ is the share represented by application a in the use of the raw candidate material
- $Subshare_{i,a}$ is the share of candidate material which is substituted by substitute material i , in application a . In other words, it is the share of $Share_a$ substituted by i .

SI_{SR} is thus a geometric average between 3 parameters, SP , SCr and SCo , weighted with respect to the share of raw materials in application a and sub-share of the substitute i in this application a . Clarifications about these parameters are given below.

- **SP** : Substitute production (SP) reflects global production of the substitute and the material as an indicator of whether sufficient amounts of substitute material are available. It reflects the market size of the candidate material compare to the one of the substitute material. The goal is that only substitutes that are available in sufficient quantities in terms of annual production are considered a potential reducing factor for the supply risk of the candidate material. The different values SP can take are presented in table G.1.

$SP = 0.8$	If the annual global production of the substitute material is higher than that of the candidate material.
$SP = 1$	If the annual global production of the substitute material is similar or lower than that of the candidate material.

Table G.1: Different values of SP [122]

- **SCr** : Substitute criticality (SCr) takes into account whether the substitute was critical in the previous EU list. Indeed It is important to assess the criticality of the substitute itself. If a substitute material is already critical, it might not be readily available as a substitute option. The different possible values of SCr are presented at figure G.2.

Substitute criticality (SCr)	Rationale
$SCr = 1$	<i>If the substitute material was on the last EU list of CRM, this material is not expected to contribute to the reduction of the SR of the candidate material.</i>
$SCr = 0.8$	<i>If the substitute material was not critical in the last EU assessment or was not screened in the previous exercise, this material is expected to contribute to the reduction of the SR of the candidate material.</i>
$SCr = 1$	<i>If no substitute material is available, no reduction of the SR is assumed.</i>

Figure G.2: Different values of SCr [122]

- **SCo** : Substitute co-production (SCo) takes into account whether the substitute is a primary product or is produced as a co-/by-product. Indeed For some materials, such as minor metals (REE , In , Ga , Ge , etc.) it could be a significant constraint on the immediate supply of these materials. The different values SCo can take are shown at figure G.3.

Substitute co-production (SCo)	Rationale
$SCo = 1$	<i>If the substitute material is mined only as a by-product or co-product — no reduction of the SR of the candidate material is assumed.</i>
$SCo = 0.8$	<i>If the substitute material is mined as a primary material — up to 20 % reduction of the SR is assumed.</i>
$SCo = 0.9$	<i>If the substitute material is mined both as a primary material, but also as a by-/co-product (e.g. the case of Molybdenum) — up to 10 % reduction of the SR is assumed.</i>
$SCo = 1$	<i>If no substitute material is available, no reduction of the SR is assumed.</i>

Figure G.3: Different values of SCo [122]

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