

École polytechnique de Louvain

Characterization for the optimization of GaN buffer

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Abstract

With the advance in telecommunication technologies, the world needs better and better power amplifiers. To this end non-conventional transistors (HEMT) have been developed. However, as they shrink in size but increase in frequency and power output, they face more and more thermal-related problems.

In this context, the goal of this thesis is to model the impact of different parameters, such as layer thicknesses, on the temperature distribution in the device. The temperature distribution is modeled using semi-analytical model using the thermal quadrupole theory and also finite element simulations. These results are then coupled to resistivity models to predict the apparition of a low resistivity parasitic channel at the bottom (AlN-Si) interface of the device.

In parallel, the "3-omega" technique was investigated. This is a technique for the measurement of the thermal conductivity of a material in a multi-layered system. It consists in a oscillating current being applied to a heater, simple rectangular metal strip on top of the sample to analyse. This generate an heat wave at double the frequency in the specimen which is then send back to the heater. This leads to an increase of the temperature at the surface. The change in temperature then induces a change in resistance of the heater due to its temperature coefficient of resistance (TCR). This variation of resistance when multiplied with the input current generates a voltage across the heater which oscillates at thrice the initial frequency.

This signal can then be picked-up by a device called a lock-in amplifier to get the thermal properties of the sample by sweeping in frequency.

Measurement validated the setup for low thermal conductivity substrate (Quartz) but it showed inconsistent results with high thermal conductivity substrate (Si). More work needs to be done to fix current issues with the setup.

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Chapter 1

Introduction

1.1 Context

With the advent of telecommunication technologies like 5G or 6G with ever-increasing data rate, range and portability, electrical components require higher working frequencies and higher output power while decreasing their size and keeping the price relatively low.

This combination of requirement leads to the use of Gallium Nitride (GaN) devices (HEMT and the likes) for two main reasons: high carrier mobility alongside a high band-gap. Compared to other materials used, GaN has in general higher power added efficiency, PAE and saturated power, P_{sat} in the working frequency of sub 6GHz and mm-wave 5G bands[1].

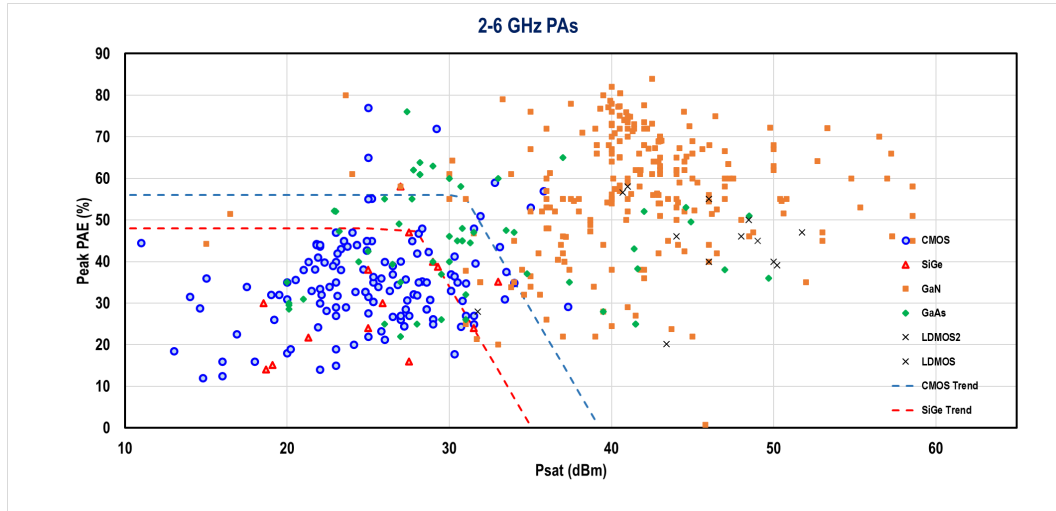


Figure 1.1: Performance trends for RF power amplifiers, considering various technologies. In the 2-6GHz band, GaN demonstrate its superiority in terms of both output power (P_{sat}) and efficiency (peak PAE). [2]

But even with good efficiency, devices still produce heat which needs to be taken care of. Self-heating is considered a major concern in RF device scaling. Moreover, as device feature sizes become comparable to the mean free path of carriers of heat (micrometer range for phonon), heat flow turn non-diffusive which worsens self-heating and complicates accurate thermal modeling. [3]

This is especially the case for thermal conductance in thin (hundreds of nanometers to 1 micron thick) films in which its value drastically reduces compared to bulk values. Also, as

the thermal conductivity of the thin films decreases, the thermal boundary resistance (TBR) becomes more noticeable to the point that it cannot be neglected when computing the total effective thermal conductance.

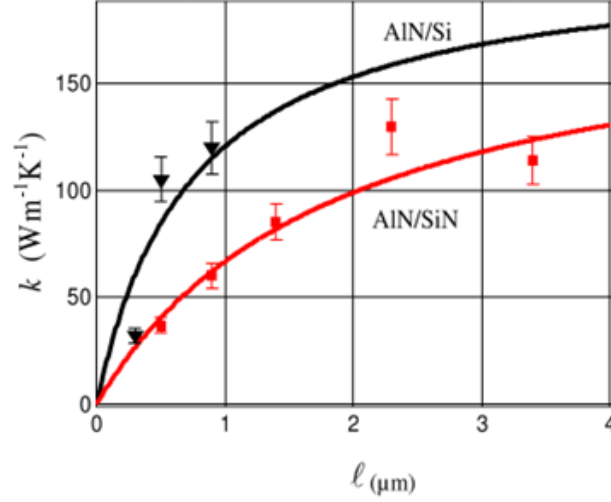


Figure 1.2: Effective total thermal conductivity (cross-plane) of AlN thin film on different substrates. It can be modeled by $l.k^{-1} = l.k_b^{-1} + G^{-1}$ with l , k , k_b and G^{-1} being the layer thickness, the total effective thermal conductivity, the bulk thermal conductivity and TBR, respectively. This demonstrates the reduction in thermal conductivity for thinning films and the growing impact of TBR. [4]

1.2 GaN (MIS)HEMT fundamentals

Gallium Nitride is semi-conductor in III-V family when in its Wurtzite crystal form. It has a band-gap $E_g \approx 3.39$ eV and a lattice constant $a \approx 3.2$ Å [5]. This lattice constant value is different than the one in Silicon, which will result in lattice mismatch when growing GaN directly on Si substrate. This coupled to the fact that they also have a different thermal coefficient (growing temperature can reach 1000°C) makes the hetero-epitaxy difficult [1].

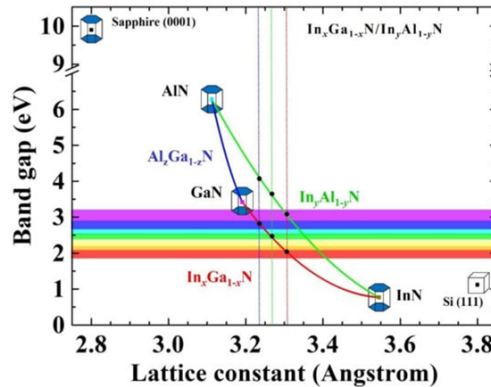


Figure 1.3: Differences in lattice and band-gap between Nitride-based semiconductors, with Silicon for reference.

This leads us to the introduction of a buffer between the channel layer and the substrate to reduce as much as possible the density of dislocations in the channel. An increase of dislocation density has been known to reduce drastically electronic mobility in semi-conductors so

we want it as low as possible, especially in High Electron Mobility Transistors (HEMT).

In practice, this is achieved by using a first nucleation layer of AlN of around 200 nm then followed by a superlattice (SL) of alternating AlN/ $\text{Al}_x\text{Ga}_{1-x}\text{N}$ with a total thickness of around 1 μm . The exact reason of each layer thickness, growth conditions, and layer composition is far beyond the scope of this thesis and thus won't be attempted to be explained. It is, as common in engineering, a game of trade-off between different KPI to have the "best" device in the end.

Si_3N_4	5 nm
AlGaN (25% Al)	15 nm
AlN 2DEG	1 nm
GaN channel	300 nm
C-GaN	1 μm
AlN / AlGaN (10% Al) superlattice	990 nm
AlGaN (30% Al)	40 nm
AlN	175 nm
Si	1150 μm

Figure 1.4: GaN HEMT buffer stack example [6]

Also, it is known that during the growth of the AlN layer, a low resistivity parasitic channel is created at its interface with the substrate [7]. To be more precise, it is situated just underneath the interface and spreads out for a few microns in the silicon layer.

This low resistivity channel is of a major concern for RF applications as it has been shown that it leads to RF substrate losses and harmonic distortions, two important problems of RF devices. As resistivity is dependent of temperature, it is important to model distribution to predict its changes based on the layer properties such as thickness.

Chapter 2

Temperature dependence of device

As previously mentioned, GaN HEMT excel in terms of RF performances, especially at higher power density. For GaN-on-Si, the saturation power level (P_{SAT}) can reach a couple of W/mm [8], which implies comparable levels of dissipated heat in the device due to inefficiencies (e.g. Joule heating). As most material properties are sensible to temperature changes, some more dramatically than others, a thermal modelling is required in order to avoid any unexpected behaviour.

GaN transistors are known to suffer from self heating [9] even on traditional substrates such as SiC which have relatively high thermal conductivity ($490 Wm^{-1}K^{-1}$). This becomes even more relevant for GaN-on-Si as silicon has a much lower thermal conductivity ($156 Wm^{-1}K^{-1}$), which results in higher temperature in the device.

In this section, the impact of various parameters on the temperature rise and its effect on the substrate will be discussed.

2.1 Simplifications to the thermal model

The device of interest is a multi-layered system in 3D with multiple escape routes for heat to flow to. Simulating the whole device and all of its details is however not possible and not optimal. Indeed, as most layer thickness are on the order of microns or lower, heat transport is no longer diffusive. This is the case as the phonon mean free path is the same range and we start to see ballistic transport instead. This means that material properties can no longer be described accurately by their bulk behaviour and boundary effects start to become non negligible. As such, assumptions and simplifications must be made to help with the modelling while achieving accurate results.

2.1.1 Taking top layers into account

As mentioned in [section 1.2](#), the system of interest is a multi-layered system with a top part (mostly insulating layers) and a bottom part (channel and below). The heat generated in the system comes from Joule heating in the channel as current flows from the drain to the source of the transistor. This current is modulated by the gate and as such, we can approximate at the first order that it is as wide and large (i.e. has the same area) as the gate above. As for the thickness, the transistor operates with a 2D electron gas (2DEG) which is located on the top interface (due to quantum effects, in reality it is located a few nanometers in the GaN layer) of the channel. This is represented in the model structure ([Figure 2.1 right](#)) as a planar heat source on top of the GaN layer.

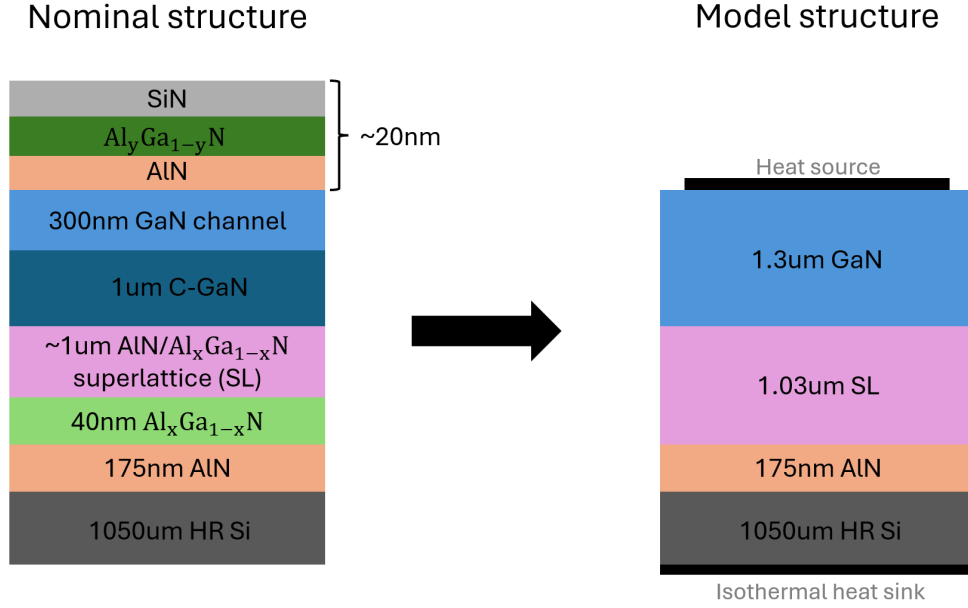


Figure 2.1: 2D cut of the device of interest before and after simplifications for thermal modelling. The GaN and C-GaN layers are combined into one. Same thing for the superlattice and the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layer. The three top-most layers are ignored as the heat is only modeled to flow from the heat source to the bottom isothermal boundary. Not to scale.

Also, as we're more interested in the substrate, the top part of the structure will be ignored. It is not to say that it plays no role in the thermal budget of real devices but it requires many more assumptions (which will not be discussed in this work) to accurately describes the behaviour of the system. To be more specific, we should model the three terminals of the transistor and a part of the back end of line as the metal lines are way better heat conductors than the layers of electrical insulator. This contribution to the temperature rise can however be modelled as a parallel conductance to the one between the heat source and the isothermal heat sink. We will approximate the former to be infinite at the first order.

2.1.2 Reducing the layer count

The C-GaN layer is similar to the layer above - an unintentionally doped¹ GaN (UID GaN, shortened as GaN) - with the difference that it is doped with carbon (hence *C*-GaN). This doping influences several properties of the material, for example thermal conductivity (which is the most relevant property in our case). The thermal conductivity of doped GaN is sensitive to the impurity concentration for high levels of doping, around 10^{20} cm^{-3} [10]², which is on the higher edge of the range of doping used. This can result in a decrease of thermal conductivity on the order of tens of percents.

Layer thickness and defects concentration, which directly depends on layer thickness [11], have a way more significant impact on thermal conductivity due to phonon interactions as mentioned at the start of this section. Due to those facts, the two GaN layers can be combined into one.

¹This particular name comes from the way GaN is grown and can be understood, albeit slightly incorrect, as undoped.

²In this paper, the effects of Mg (and other dopants) is discussed. C has a similar doping effect, but forms substitutional defects on N sites, instead of Ga sites for Mg. This may increase/decrease the threshold value, improving/degrading the thermal conductivity compared to the Mg case.

The 40 nm of $\text{Al}_x\text{Ga}_{1-x}\text{N}$ can be merged with the superlattice to form an unique layer, as the latter is formed of alternating AlN and $\text{Al}_x\text{Ga}_{1-x}\text{N}$. The ternary alloy layers in the superlattice have a similar thickness compared to the single layer which makes the difference even more negligible from a thermal standpoint.

Furthermore, due to presence of ternary alloy and the layers being so thin, the heat propagation is heavily limited by alloy scattering, which once again makes the model layer more uniform.

All in all, this reduces the layer count to only four layers, one of which - the substrate (HR Si) - is way thicker than the rest and retains its bulk behaviour.

2.2 Heat equation

Before delving any deeper in the simplifications and going to the analysis, we have to properly set up the problem. As stated before, we want to know the temperature distribution in the (3D) device, starting from a ambient temperature T_0 , knowing that we have an 2D influx of heat from the top and that we can dissipate heat via a heat sink at the bottom ([Figure 2.1](#)).

The relationship between heat transfer and temperature is stated in Fourier's law of heat conduction:

$$\vec{q} = -k\vec{\nabla}T, \quad (2.1)$$

where:

- $\vec{q}$ is the heat flux density in $[\text{W}/\text{m}^2]$
- k is thermal conductivity (diagonal 3x3 matrix) in $[\text{W}/\text{m.K}]$
- T is the temperature in $[\text{K}]$

k is usually treated as a scalar as most materials have an isotropic thermal conductivity or one which is close enough to be approximated as such. It will be shown later that this assumption cannot be made in this work. As such, we will write the thermal conductivity as the following:

$$k = \begin{pmatrix} k_{//} & 0 & 0 \\ 0 & k_{//} & 0 \\ 0 & 0 & k_{\perp} \end{pmatrix}, \quad (2.2)$$

where $k_{//}$ and $k_{\perp}$ are the in-plane (x and y) and cross-plane (z) thermal conductivity respectively. This distinction between in- and cross-plane is reminiscent of the fact that the GaN layer, superlattice and AlN layer all have a very low thickness. For the substrate, its thermal conductivity is isotropic (i.e. $k_{//} = k_{\perp}$).

From Fourier's law, a second order partial differential equation can be derived to describe the evolution of temperature is time and space:

$$\rho c_p \frac{\partial T}{\partial t} = \vec{\nabla} \cdot (k\vec{\nabla}T) + q_V, \quad (2.3)$$

where:

- q_V is the volumetric heat generation [W/m³]
- ρ is density [kg/m³]
- c_p is the specific heat capacity [J/kg.K]

One can see that [Equation 2.3](#) is a linear equation. So, using the substitution $T = T_0 + \Delta T$ and setting $q_V = 0$ (as we don't have any heat source *in* the model structure), we have:

$$\rho c_p \frac{\partial \Delta T}{\partial t} = k_{//} \left(\frac{\partial^2 \Delta T}{\partial x^2} + \frac{\partial^2 \Delta T}{\partial y^2} \right) + k_{\perp} \frac{\partial^2 \Delta T}{\partial z^2}. \quad (2.4)$$

Indeed, as T_0 is constant over space and time (by definition) we only need to take into account the temperature rise. Also, we can further split the temperature $\Delta T = \Delta T_{DC} + \Delta T_{AC}$, the former not depending on time.

So for steady-state (DC) we have:

$$\frac{\partial^2 \Delta T_{DC}}{\partial x^2} + \frac{\partial^2 \Delta T_{DC}}{\partial y^2} + \frac{k_{\perp}}{k_{//}} \frac{\partial^2 \Delta T_{DC}}{\partial z^2} = 0 \quad (2.5)$$

This last equation is the basis of what will be discussed in this section onwards. The AC part of [Equation 2.4](#) (which keeps the same form) will be discussed in [chapter 3](#).

2.2.1 Boundary conditions

There's three type of boundary condition relevant for this system:

- Isothermal boundary: a 2D boundary on which temperature is set to a known value.
- Adiabatic boundary: a 2D boundary on which the normal heat flux is null. This can be interpreted as either a perfect thermal insulation, or a perfect thermal mirror.
- Heat source: a 2D boundary on which heat flux density is set (normal to the boundary surface).

The different boundary conditions have been represented on the schematic below:

While the boundary conditions on the heat source and the heat sink are intuitive, the adiabatic boundary condition seems to come out of nowhere. To be more specific, the one on the same plane as the heat source is easily understood as no heat going up due to what was discussed earlier (treating top and bottom separately). But the one on the vertical "walls" (right and left boundaries on [Figure 2.2](#)) makes as much sense as the existence of those "walls" in the first place.

Those "walls" are simply artefacts of numerical analysis. In a perfect (theoretical) world, the medium would go on forever in both in-plane directions (x and y), requiring no boundary conditions at the edge as this edge would simply not exist. Even in the real world, this edge, which exists, isn't of concern as it is too far from the region of interest and this approximation of infinite medium is correct. But when turning to numerical methods, one requires a finite domain. Those walls only exists as a constraint of the need to define a finite region of interest for numerical analysis. Thus, boundary conditions are needed for those new surfaces which lack any physical meaning.

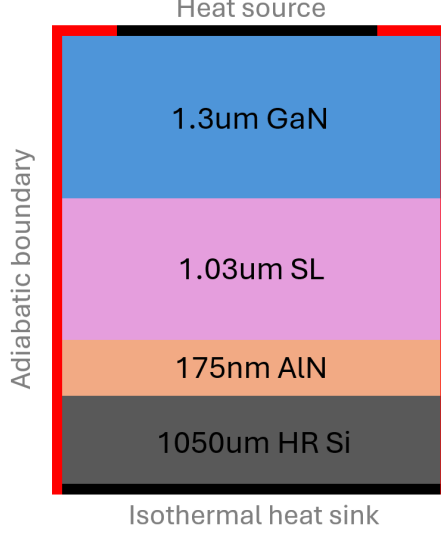


Figure 2.2: 2D slice of thermal model structure with boundary conditions. Not to scale.

However, the best boundary condition for them would be to simply let heat go through without any impact, as they shouldn't exist in the first place. Designing such boundary condition is hard task and all current attempts always reflect part of the incoming quantity of interest (in our case, heat). A simple solution to this problem, which is commonly chosen, is to apply a boundary condition which is easy to compute and make the domain as large as required in the problematic directions. This simple boundary condition is the adiabatic boundary condition.

This poses a problem: the bigger the domain is, the more computation the problem will require to be solved. This is especially true if the magnitude of the heat spread doesn't decrease fast enough, i.e. we need a high aspect ratio between the in-plane and cross-plane direction to alleviate the artefacts of the non-physical walls.

2.2.2 Symmetries

As shown on [Figure 2.3a](#), the base model structure is a rectangular prism with variation (in thermal conductivity) in the cross-plane direction, with a small rectangle (heat source) carved in its top face.

There is some obvious symmetry planes in the structure as highlighted on [Figure 2.3b](#). We can remove from the simulation domain one side each symmetry plane without loss of information (by symmetry). This removal results in the simplified model structure shown on [Figure 2.3c](#).

By dividing the simulation domain in 4 regions (and keeping only one), we introduced two new boundaries. Those require boundary conditions which are, fortunately, pretty straight-forward.

As stated before, adiabatic boundaries act as perfect thermal mirror, which is what we have here. Mathematically, we have at one of those plane that the temperature on one side $T_+ = T(\vec{p}_0 + \delta\vec{n})$, with $\vec{p}_0$ a point on the symmetry plane, $\vec{n}$ the normal vector to that plane and δ some strictly positive real number. On the other side, we have $T_- = T(\vec{p}_0 - \delta\vec{n})$. But, by definition of $\vec{n}$ and the symmetry plane, we know that those two temperatures are equal, such that the following equality holds even in the limit:

$$\lim_{\delta \rightarrow 0} \frac{T_+ - T_-}{2\delta} = \vec{\nabla} T(\vec{p}_0) \cdot \vec{n} = 0. \quad (2.6)$$

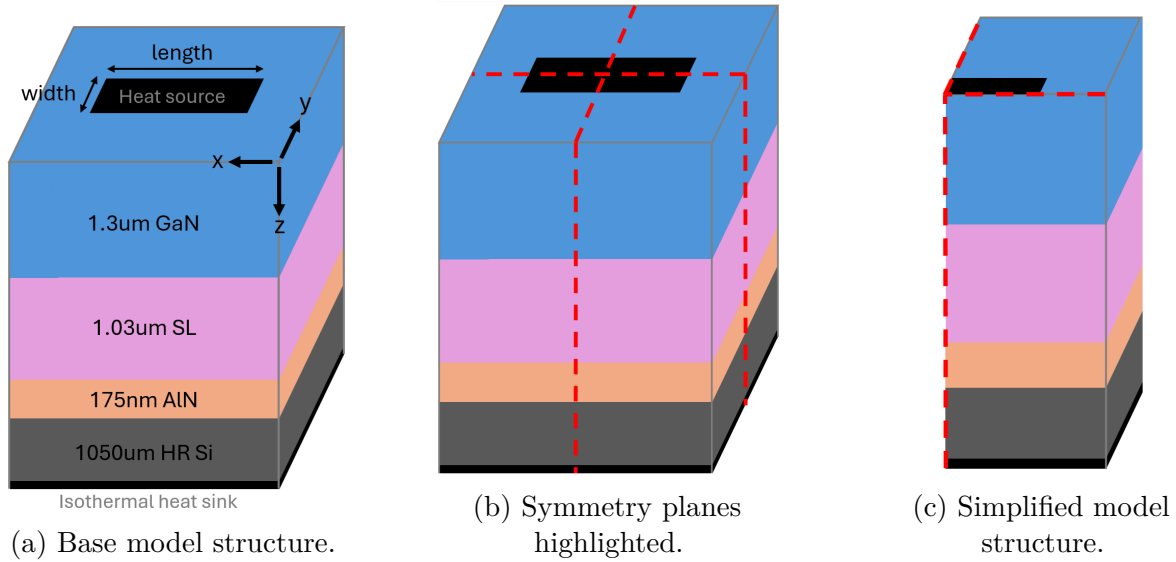


Figure 2.3: Simplification of the base model structure by taking into account symmetries.
Not to scale

Using Fourier's law ([Equation 2.1](#)), we get that there's no heat flux in the direction of the normal to a symmetry plane, hence the adiabatic boundary condition.

2.2.3 Coordinate system

To simplify notations, the center of the heat source will be considered as the origin. As shown on [Figure 2.3a](#), the x coordinate is oriented along the length of the heat source, the y coordinate along its width and the z coordinates indicates the depth in the layer stack.

2.3 What needs to be solved

Now that we have a correct set of equation, boundary conditions and simulation domain, we need to define the precise quantity that we wish to get. We can (and will) compute the temperature distribution in the whole device, but not every bit of information is relevant. We need metrics to compare results between themselves to try and find a set of solutions.

Note that due to the linearity of the heat equation, we're solving for a temperature rise relative to the environment. A convenient choice of temperature reference would be 300K or 0. The later as been chosen for convenience sake as the temperature of the isothermal heat sink. This ensure that the temperature computed is the temperature rise due to the heating and not the "true" temperature. This means that the true temperature needs to be computed in post. While this requires another step to be made after running a simulation, it makes the scaling of the solution easier.

The first reason is that the temperature rise is normalized by the input heat flux density. Again, due to the linearity of the equations, the temperature rise is linear with the input heat (i.e. 2x heat gives 2x temperature rise). If we work with temperature rise instead of absolute temperature, we can simply multiply the output of the simulation by the input (minding units) then add the reference temperature.

The second reason is that we can reuse without worry output data for different substrate conditions. While it's common to use normal temperature conditions ($T = 300\text{K}$), devices

are usually never alone on a chip. This results in a substrate temperature which can be significantly higher (e.g. $T = 475\text{K}$). It is then better to stay with temperature rise instead of absolute temperature to avoid any confusion in the post processing.

From now on, the words "temperature rise" will be shortened to "temperature" when talking about the output of a simulation before any post-processing.

2.3.1 Temperature rise in the heat source

The most obvious metric is the average temperature of the heat source. While computing the temperature only at the center of the heat source is (slightly) faster, we're interested in what happens in the whole channel (which is the heat source) as it will have an impact on its properties (e.g. carrier mobility).

This value computed by simply averaging the temperature over the heat source:

$$\bar{T} = \frac{\int_{\Omega_H} T(x, y, 0) d\Omega}{S_H}, \quad (2.7)$$

where Ω_H is the heat source and S_H its area, computed as $\int_{\Omega_H} d\Omega$.

2.3.2 Temperature rise at the AlN-Si interface

The different layers between the channel (heat source) and the substrate being good insulators [5]. On top of that, material engineering done in the layer stack, as discussed in [section 1.2](#), makes the leakage current through the substrate negligible. Thus, the main problem that can arise is substrate loss when the resistivity of the substrate decreases dramatically, going from kilo-ohms to tens of ohms.

This is mostly due to the spontaneous generation of carriers in silicon by the rise of temperature. This will be discussed in more details later on. This means that we have to monitor the temperature profile in the whole substrate. However, as the heat source is not infinitely wide and located on the top of the device, we can expect the temperature distribution to depend on both in-plane and cross-plane directions. In other words, the resistivity in the silicon layer will vary with each dimension in a possibly complex pattern (due to the layers above).

As such, we should define a quantity which takes those changes in resistivity while reflecting their relative proximity with the heat source. One such metric is called the effective resistivity. It is a common figure of merit used to compare RF substrate performance using CPW line measurement [12]. This consists in modelling the possibly complex structure below the CPW line as homogeneous substrate of uniform dielectric constant $\epsilon_{r,eff}$ and resistivity ρ_{eff} . The latter is called effective resistivity.

Computing this value is non-trivial as one needs to model the propagation of the electromagnetic field through the stack. To make things worse, this highly depends on cross CPW line dimensions and frequency.

Combining those factors with a lack of time, the chosen metric was simpler: the temperature at the AlN-Si interface. However, contrary to the previous metric, this one is not an average. The reason behind this choice is that as we go deeper in the layers, the heat tends to spread which results in a less localized temperature distribution in the in-plane directions. This makes the choice the choice of an averaging domain less obvious. Also, as stated just before

with the effective resistivity, one should look for the electromagnetic field distribution, which also tends to spread out when allowed to. However, it will chose the path of least resistance.

Intuitively, the temperature should be greater the farther we are from the heat sink and the closer we are from the heat source. Hence the highest temperature in the substrate should be at the interface with AlN right under the heat source. It will be shown later that higher temperature results in lower resistivity. This translates into a conductive parasitic channel right at that interface which will focus the electromagnetic field and lower the effective resistivity. Thus, monitoring the temperature there gives a good insight in the performance of the substrate.

2.4 Solving the heat equation

Using [Equation 2.5](#) we can look at a simple solution (mono-layer with point source) to get a feeling on what the solution will look like.

2.4.1 Parallel with electricity

Before going any further, an analogy between thermal modeling and electricity needs to be introduced. This can give a better insight in further explanations.

Just as flux of charges (current I) through a electrically resistive material (resistor R) induces an electrical potential (V), a heat flow (Q) through a thermally resistive material (thermal resistance R_{th}) induces a difference in temperature (T):

$$V = RI \quad (2.8)$$

$$T = R_{th}Q. \quad (2.9)$$

The value of those resistances depends on their geometry. A useful simple case is the prism with cross section S and height L , such that:

$$R = \rho \frac{L}{S} \quad (2.10)$$

$$R_{th} = k \frac{L}{S}. \quad (2.11)$$

This can be intuitively understood as a larger cross section gives more room the current (heat flow) to go through the material, resulting in decreased resistance. But on the contrary if the current (heat flow) needs to travel a longer distance (i.e. bigger height), the voltage drop (temperature difference) will be higher.

Due to the linearity of the heat equation, one can compute an equivalent resistance for a whole system to get the temperature as a function of the supply heat. [Equation 2.11](#) may no longer work in that case.

2.4.2 1D case

If the heat flow is restricted to the cross-plane direction (i.e. the heat source spans the whole in-plane directions for a certain z), we can directly solve the heat equation, even for the multi-layered system.

$$\frac{\partial^2 \Delta T_{DC}}{\partial z^2} = 0 \Rightarrow \Delta T_{DC}(z) = Az + B. \quad (2.12)$$

Combining Equation 2.12 with Equation 2.1, we see that each layer simply acts as a thermal resistance, in series with the others as the layers are stacked:

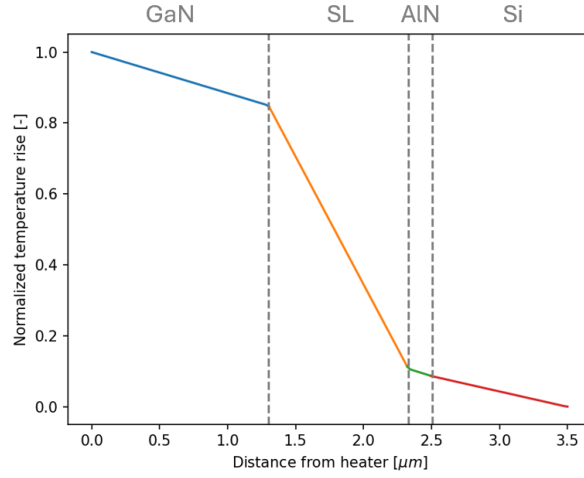


Figure 2.4: Temperature distribution in the full stack in 1D. Here the Si layer is only 1μm thick.

Note that in Figure 2.4 the thickness of the Si layer has been drastically reduced to see what happens in the top layers, because $R_{th} = k_{1D}L$ in 1D (assuming that k_{1D} doesn't depend on the layer thickness). Going to the full 1050μm of Si doesn't change the circuit as we would just need to add a series R_{th} with the missing thickness, which just changes the temperature values in an additive fashion (i.e. $\Delta T_{DC} = \Delta T_{top} + \Delta T_{Si}$).



Figure 2.5: 1D thermal equivalent circuit for the model structure.

The value of the 1D-equivalent thermal conductivity k_{1D} is simply the value for the 3D one, divided by the surface area of the heat source (e.g. 1m^2).

2.4.3 3D case (semi-analytical)

Now as the heat has access to in-plane dimensions, we should expect the thermal resistance to drop compared to the 1D case as the heat can spread out, increasing its cross-sectional area the deeper it propagates in the structure.

Taking the Laplace transform of the in-plane coordinates ($x \rightarrow \xi$, $y \rightarrow \zeta$) of Equation 2.5 [13], we get:

$$\frac{\partial^2 \hat{T}}{\partial z^2} = \beta^2 \hat{T} \quad (2.13)$$

$$\beta = \sqrt{\frac{k_{//}}{k_{\perp}}(\xi^2 + \zeta^2)}. \quad (2.14)$$

Equation 2.13 tells us that we can *easily* compute the temperature distribution in the cross-plane direction if we know its distribution in the in-plane directions: we can just take its Laplace transform and propagate it with the differential operator.

Note that a hat on top of a variable means that we have taken its Laplace transform over the in-plane coordinates ($\Delta T \rightarrow \hat{T}$ for better readability).

Combining Equation 2.13 with Equation 2.1, we get the matrix formalism:

$$\begin{bmatrix} \hat{T}_{in}^{(l)} \\ \hat{q}_{in}^{(l)} \end{bmatrix} = \underbrace{\begin{bmatrix} \cosh(\beta_l d_l) & \frac{1}{\kappa_{\perp,l} \beta_l} \sinh(\beta_l d_l) \\ \kappa_{\perp,l} \beta_l \sinh(\beta_l d_l) & \cosh(\beta_l d_l) \end{bmatrix}}_{M^{(l)}} \begin{bmatrix} \hat{T}_{out}^{(l)} \\ \hat{q}_{out}^{(l)} \end{bmatrix} \quad (2.15)$$

$$M^{(l)} = \begin{bmatrix} M_{11}^{(l)} & M_{12}^{(l)} \\ M_{21}^{(l)} & M_{22}^{(l)} \end{bmatrix}, \quad (2.16)$$

where $M^{(l)}$ is the 'thermal quadrupole' matrix (TQM), β_l is the Laplace parameter (Equation 2.14), d_l is the layer thickness and l is the current layer.

The inlet/outlet (for $\hat{T}_j^{(l)}$, $\hat{q}_j^{(l)}$) are shown on the following figure:

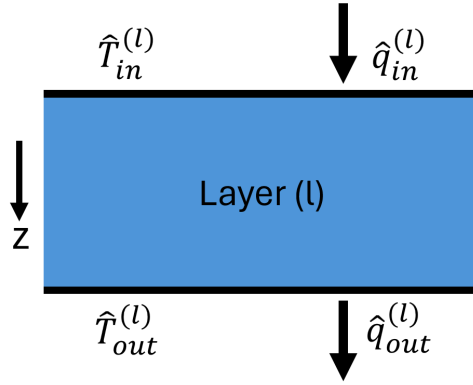


Figure 2.6: Schematic of the inlet/outlet of a single layer in the matrix formalism.

This means that we can model our (simplified) structure as a concatenation of TQMs to get the temperature on the surface knowing the heat dissipation input [14]³:

$$\begin{bmatrix} \hat{T}_{surface} \\ \hat{q}_{surface} \end{bmatrix} = \underbrace{\begin{bmatrix} M_{11}^{(1)} & M_{12}^{(1)} \\ M_{21}^{(1)} & M_{22}^{(1)} \end{bmatrix}}_{M^{GaN}} \cdot \underbrace{\begin{bmatrix} M_{11}^{(2)} & M_{12}^{(2)} \\ M_{21}^{(2)} & M_{22}^{(2)} \end{bmatrix}}_{M^{SL}} \cdot \underbrace{\begin{bmatrix} M_{11}^{(3)} & M_{12}^{(3)} \\ M_{21}^{(3)} & M_{22}^{(3)} \end{bmatrix}}_{M^{AlN}} \cdot \underbrace{\begin{bmatrix} M_{11}^{(4)} & M_{12}^{(4)} \\ M_{21}^{(4)} & M_{22}^{(4)} \end{bmatrix}}_{M^{Si}} \cdot \begin{bmatrix} \hat{T}_{sink} \\ \hat{q}_{sink} \end{bmatrix}. \quad (2.17)$$

Note that in this model the interfaces are considered ideal, i.e. there's no increase in temperature as the heat passes through the interface between two layer. This resistivity can be modeled once again as a TQM which is concatenated between the TQMs of a pair of layers:

$$\begin{bmatrix} \hat{T}_{in}^{(l)} \\ \hat{q}_{in}^{(l)} \end{bmatrix} = M^{(1)} \cdot \underbrace{\begin{bmatrix} 1 & r \\ 0 & 1 \end{bmatrix}}_{M^{interface}} \cdot M^{(2)} \cdot \begin{bmatrix} \hat{T}_{out}^{(l)} \\ \hat{q}_{out}^{(l)} \end{bmatrix}, \quad (2.18)$$

³This is the subject of a simulation tool by Bjorn Vermeersch, which I was permitted to use.

where $M^{\text{interface}}$ is the TQM representing the interface and r is the value of the interface resistivity (in $[\text{K.m}^2/\text{W}]$).

Computing the effective value of this interface resistivity for each pair of layers is beyond the scope of this master thesis and will thus not be taken into account as its effects are almost negligible in our case. Setting $r = 0$ in the above equation leads to the interface TQM to be equal to the identity matrix, so we can just leave it out of the equations for better readability.

If we inspect Equation 2.17 in detail, we see that M^{system} can be easily computed by going through the layers one at a time, starting from the bottom (Si) layer⁴. Also, the value of $\hat{q}_{\text{surface}}$ and $\hat{T}_{\text{sink}}$ are known. They are respectively the heat source profile on the surface (which will be approximated as a simple 2D step function) and the temperature of the heat sink, which was chosen to be 0. To be more precise, q_{surface} has the form:

$$q_{\text{surface}}(x, y) = \begin{cases} q & \text{if } |x| \leq \frac{w_x}{2} \text{ and } |y| \leq \frac{w_y}{2} \\ 0 & \text{otherwise} \end{cases}, \quad (2.19)$$

where w_x is the length of the rectangular heat source and w_y its width (as shown on Figure 2.3a). This leads its Laplace transform $\hat{q}_{\text{surface}}$ to be:

$$\hat{q}_{\text{surface}}(\xi, \zeta) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{A_{mn}}{W_x W_y} \frac{\sin(\xi_m w_x / 2)}{\xi_m} \frac{\sin(\zeta_n w_y / 2)}{\zeta_n} \quad (2.20)$$

$$A_{mn} = 4p_0(2 - \delta_{m0})(2 - \delta_{n0}) \quad \xi_m = \frac{2\pi m}{W_x} \quad \zeta_n = \frac{2\pi n}{W_y}, \quad (2.21)$$

where p_0 is power density of the heat source $[\text{W}/\text{m}^2]$ and δ_{ij} is the Kronecker delta ($\delta_{ij} = 1 \Leftrightarrow i = j$, and 0 if $i \neq j$).

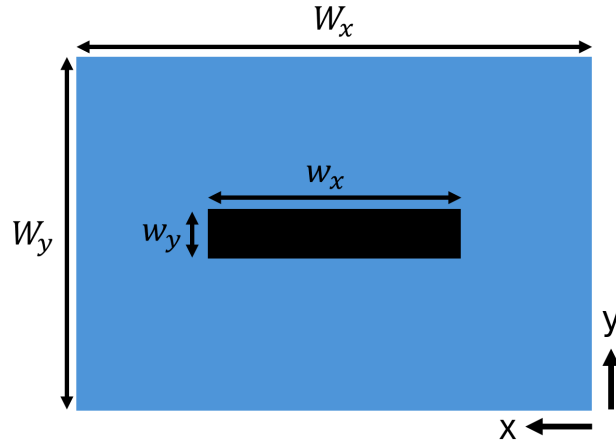


Figure 2.7: Top side view of the structure with the different length annotated. The black rectangle represents the heat source.

⁴It is customary in linear algebra to perform concatenation from the left side, i.e. apply M^{AlN} on M^{Si} from the left. This is however not mandatory and we could as well start with M^{GaN} , apply M^{SL} from the right, ... This is just a matter of convention and both of them are similarly expensive to compute.

The two lengths W_x and W_y correspond to the side-lengths of the domain of simulation (as discussed in [subsection 2.2.1](#)). Their value will directly affect the output value of any simulation and also its efficiency.

Indeed, as the simulation box decreases in size we get more artefacts as the boundary conditions on the related walls are not perfect. But simulating more takes exponentially more resources, potentially for nothing. Those walls are still simulated as perfectly adiabatic, but are in fact just a periodic condition on the solution (which is equivalent).

In that regard, we need to truncate the infinite sums in [Equation 2.20](#) with regards to W_x , W_y , w_x and w_y . This comes from the fact that those 4 quantities define the mesh and its required precision (aka grid cell size).

Empirically, a good set of values is as follow:

$$N_\xi \approx 5 \frac{W_x}{w_x}, \quad N_\zeta \approx 5 \frac{W_y}{w_y}, \quad (2.22)$$

such that

$$\hat{q}_{surface}(\xi, \zeta) = \sum_{m=0}^{N_\xi} \sum_{n=0}^{N_\zeta} \frac{A_{mn}}{W_x W_y} \frac{\sin(\xi_m w_x / 2)}{\xi_m} \frac{\sin(\zeta_n w_y / 2)}{\zeta_n}. \quad (2.23)$$

The leading coefficients in [Equation 2.22](#) (5) are there to limit the error when truncating the infinite sums, which tends to smooth out the discontinuous nature of the step function.

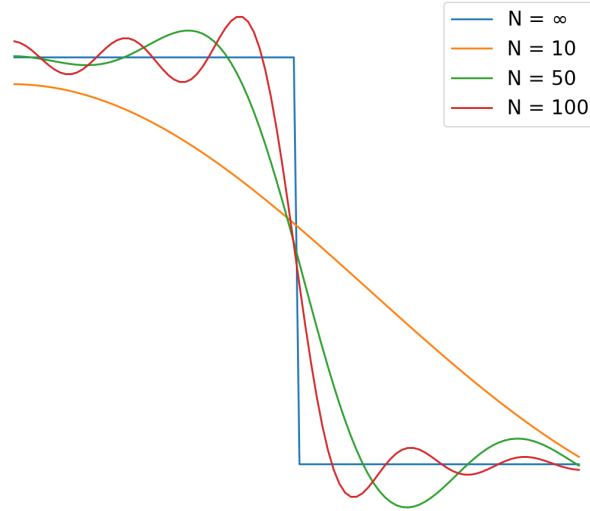


Figure 2.8: Approximation of a window function (1 if in domain, 0 elsewhere) with varying number of Fourier coefficients. The lower number of coefficients we take, the more spread out is the resulting approximation.

As shown in [Figure 2.8](#), we need to take as much coefficients as possible to avoid the profile of the heat source to spread out. Again, this is a trade-off with the simulation size as the finer the grid, the more computation required to do.

Going back to [Equation 2.17](#), the two left unknowns are the temperature distribution at the surface ($\hat{T}_{surface}$) and the heat distribution at the isothermal sink ($\hat{q}_{sink}$). The later can give us insights in the footprint of a device, which is useful when putting lots of devices side by side (i.e. knowing what the minimum spacing between them is). In the context of this master thesis, only the former is relevant to look at.

As such, with some algebra, one can show that $\hat{T}_{surface}$ is related to $\hat{q}_{surface}$ in the following manner:

$$\hat{T}_{surface}(\xi, \zeta) = \frac{M_{11}^{system}(\xi, \zeta) + h_{sink} M_{12}^{system}(\xi, \zeta)}{M_{21}^{system}(\xi, \zeta) + h_{sink} M_{22}^{system}(\xi, \zeta)} \hat{q}_{surface}(\xi, \zeta). \quad (2.24)$$

In our case, the convection coefficient defined as $h_{sink} = \hat{q}_{sink}/\hat{T}_{sink}$ is approximated to be infinite (perfect isothermal sink) such that Equation 2.24 becomes:

$$\hat{T}_{surface}(\xi, \zeta) = \frac{M_{12}^{system}(\xi, \zeta)}{M_{22}^{system}(\xi, \zeta)} \hat{q}_{surface}(\xi, \zeta). \quad (2.25)$$

As only the ratio of coefficients of the TQM are involved, we can multiply any sub-TQM by a (non-zero) arbitrary coefficient. One such choice is to divide by $\cosh(\beta_l d_l)$ to improve the numerical stability of the intermediate computations:

$$M'^{(l)} = \begin{bmatrix} 1 & \frac{1}{\kappa_{\perp, l} \beta_l} \tanh(\beta_l d_l) \\ \kappa_{\perp, l} \beta_l \tanh(\beta_l d_l) & 1 \end{bmatrix}. \quad (2.26)$$

To get the temperature rise, or at least its average over the heat source at the surface, we need to transform the value obtained in Equation 2.25 back from the Laplace domain to the initial domain.

Using the fact that we have a symmetric domain (i.e. the power density follows $p(x, y) = p(|x|, |y|)$), we get:

$$\Delta T_{surface}(x, y) = \sum_{m=0}^{N_\xi} \sum_{n=0}^{N_\zeta} \hat{T}_{surface}(\xi_m, \zeta_n) \cos(\xi_m x) \cos(\zeta_n y). \quad (2.27)$$

Integrating Equation 2.27 over the heat source surface and dividing by the surface (i.e. taking the average), we get:

$$\bar{T} = \frac{4}{w_x w_y} \sum_{m=0}^{N_\xi} \sum_{n=0}^{N_\zeta} \hat{T}_{surface}(\xi_m, \zeta_n) \frac{\sin(\xi_m w_x/2)}{\xi_m} \frac{\sin(\zeta_n w_y/2)}{\zeta_n} \quad (2.28)$$

2.4.4 3D case (FEM)

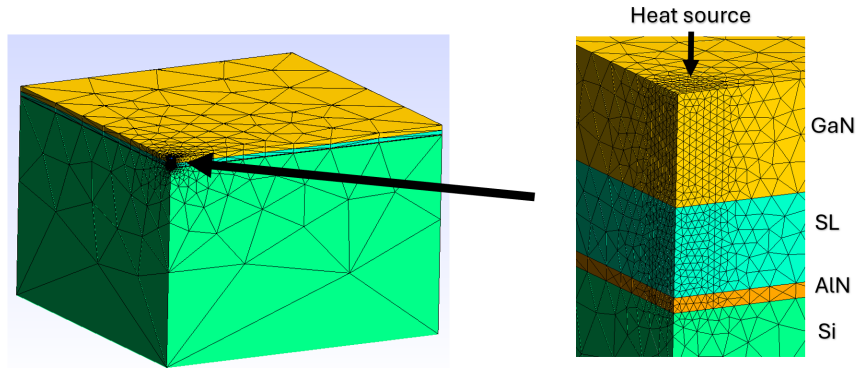


Figure 2.9: Example of a 3D unstructured mesh for a Quanscient simulation with a zoom on the right. In this example the heat source is a $1\mu m \times 1\mu m$ square.

Due to the configuration of the problem and the limitations of the matrix formalism, getting the temperature profile deeper into the stack is hard. A *simple* way around it is to use a common PDE-solving technique such as the finite element method (FEM).

As discussed before ([section 2.2](#)), the set of equations to solve here is relatively simple. It would be possible to re-implement this in programming language such as Matlab, python or even C, given a correct set of libraries. But as this is very time consuming (especially due to the boundary condition which is the heat source) and the heat equation is very well known, it is better to not reinvent the wheel.

Commercially available software's such as Matlab contain already modules capable of solving it with a variety of boundary conditions.

In the case of this thesis, the simulation software Quanscient was used.

This software can work either with a GUI or in full script mode (only code). To get a maximum of flexibility, the second option was chosen.

The pipeline to setup and solve a heating problem is as follow:

1. Provide a mesh, its dimension (1D, 2D or 3D) depending on the user's needs.
2. Assign materials with different properties to each of the region of the mesh.
3. Set up the equations to solve (i.e. the already implemented heat equation).
4. Set up the boundary conditions.
5. Tell the solver to solve for the field of interest (i.e. the temperature field).
6. Compute the relevant quantities (i.e. the temperature profile along the depth).

This is relatively easy to do thanks to Quanscient's scripting API and a simulation runs in the tens of seconds (on a default Quanscient-provided CPU) for mesh size in the order of $\sim 5k$ nodes for $\sim 80k$ tetrahedral elements.

The (3D) mesh is constructed using the built-in geometry kernel of **GMSH** and generated (and optimized) again with GMSH. The code for generating the mesh is put in .

The mesh is divided in 4 regions corresponding to the 4 layers with 3 sub-regions: the isothermal sink (bottom layer), the heat source (small rectangle on the top surface) and the high detail region in the 3 first layers (GaN, SL, and AlN) just under the heat source. Each 3D (sub-)region has a corresponding maximum element size, dictating the maximum side-length of the elements in the region.

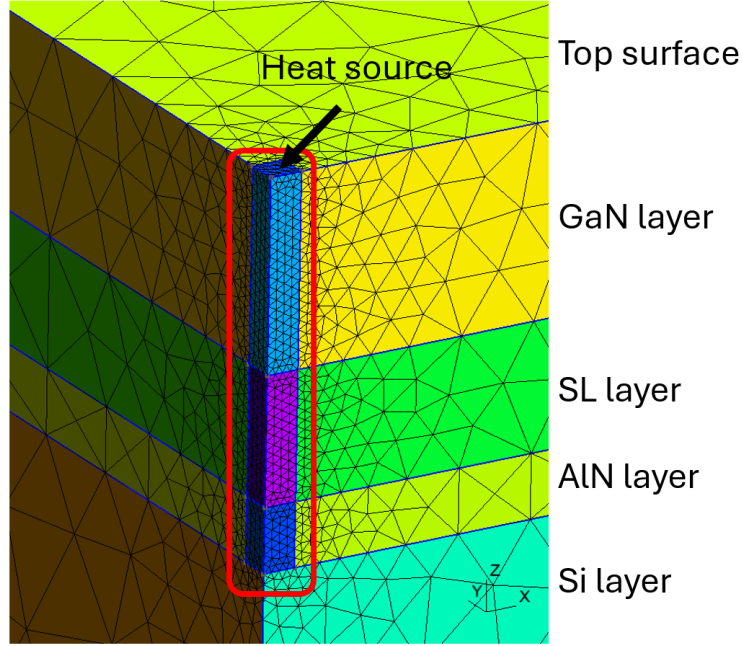


Figure 2.10: Regions in the 3D mesh for the FEM model. The rectangular prism region circled in red is the high detail region.

2.4.5 Meshing-related issues

As mentioned before, even in the case of the matrix formalism a mesh is required. It is a 2D structured grid which represents the in-plane coordinates in the Laplace domain. Its size and precision is dictated by the feature present on the top surface (heat source) and the thickness of the whole device. This last contribution comes from the natural spreading of the heat when going deeper in the device. This directly dependant on the ratio $\kappa_{//}/\kappa_{\perp}$. The higher it is, the more the heat spreads in the in-plane directions, the bigger the mesh is required for a same device thickness.

This is a problem as the device is $\sim 1050\mu m$ thick while the heat source is only $1\mu m$ wide. Empirically, the simulation box needs to be ~ 100 times greater in size than a feature in its axis. This means, taking the spreading into account, that we have to take a simulation box as wide as $100mm$ while having a sub-micrometer resolution (at least in the y direction).

Using Equation 2.22 ($w_x = 100\mu m$, $w_y = 1\mu m$ and $W_x = W_y = 100mm$), we get $N_{\xi}N_{\zeta} = 2.5 \cdot 10^9$ mesh nodes, which is *huge*. Remember that we have to make as much 2x2 matrix multiplication as there is nodes, multiplied (approximately) by the number of layers. From a computation stand-point, this number of operations is not a problem per-say, only a matter of tens of seconds instead of less than one for one run, if the program can run at all. The real problem is memory, as we would need to allocate huge arrays (in the order of giga-bytes). And so, strategies for decomposing the problem in subsets of nodes and compute their solution separately to combine them into the final one (in a divide and conquer manner) would be required, which is non-trivial to implement.

This problem resulting from the structured nature of the 2D mesh is less impacting in the FEM case, as we can use unstructured meshes there. This means that we can simulate the full thickness of the device using this method. There is still a problem, at least in 3D, as the aspect ratio of the upper layers is quite extreme ($\sim 1\mu m$ thick but several millimeters wide) resulting in a high number of tetrahedrons, or ill-shaped ones. Choosing

between a large computational effort or possibly wrong results (depending on the run parameters) is bad so another solution is required to get the impact of the full Si layer thickness.

A solution to this problem is to simulate, in FEM, only two dimensions instead of three. This can be done as the length of the heat source is way larger than its width, resulting in an almost 2D heat flow, with some edge effects. Those edge effects, which should be taken into account, disappear with the deletion of the third dimension, which is non-negligible (this will be discussed later). We can somewhat alleviate this problem by simulating both in-plane dimensions in the semi-analytical model, at the cost of reduced Si layer thickness.

Using that information, we can start by computing the temperature rise at the top of the heater using the matrix formalism, then compute the temperature profile using FEM and then combine the two results to get the temperature rise at the heater.

The first simulation will be done with a thinner Si layer with both in-plane dimensions while the second will run with the full layer thickness and without the dimension along the length of the heat source.

2.4.6 Merging results

As mentioned just before, we need a way to combine the results from a $50\mu m$ thick (Si layer) simulation with a $1050\mu m$ one. This is, luckily, almost trivial to do.

To start, we need to put labels on some quantity. We will denote d_{50} the depth (in the Si layer) which is $50\mu m$ below the AlN-Si interface, ΔT_{50} the difference in temperature between the top surface and this depth centered by the heat source (i.e. on the vertical cut line in [Figure 2.3c](#)), ΔT_{Si} the difference in temperature between d_{50} and the isothermal heat sink and $\Delta \tilde{T}(d)$ the normalized temperature rise at any depth d (1 at the heat source, 0 at the isothermal heat sink). Also, if we define $\Delta T_{\max}$ as the temperature rise in the center of the heat source and $\Delta T(d)$ the temperature rise at any depth, we have the following relationships:

$$\Delta T(d) = \Delta T_{\max} \Delta \tilde{T}(d) \quad (2.29)$$

$$\Delta T_{Si} = \Delta T(d_{50}) \quad (2.30)$$

$$\Delta T_{50} = \Delta T_{\max} - \Delta T_{Si}. \quad (2.31)$$

We can define a last quantity $\Delta \tilde{T}_{50} = \Delta \tilde{T}_{\max} - \Delta \tilde{T}_{Si} = \Delta \tilde{T}(0) - \Delta \tilde{T}(d_{50}) = \Delta T_{50} / \Delta T_{\max}$, which is the normalized temperature rise between the top surface and the depth d_{50} . Knowing that $\Delta \tilde{T}(0) = 1$ (by definition), we can compute $\Delta T_{\max}$ as follows:

$$1 - \Delta \tilde{T}(d_{50}) = \frac{\Delta T_{50}}{\Delta T_{\max}} \quad (2.32)$$

$$\begin{aligned} &\Updownarrow \\ \Delta T_{\max} &= \frac{\Delta T_{50}}{1 - \Delta \tilde{T}(d_{50})}. \end{aligned} \quad (2.33)$$

Combining [Equation 2.29](#) and [Equation 2.33](#) we can get the temperature rise in the full device using the results of the two simulations:

$$\Delta T(d) = \frac{\Delta T_{50}}{1 - \Delta \tilde{T}(d_{50})} \Delta \tilde{T}(d). \quad (2.34)$$

ΔT_{50} is obtained with the matrix formalism while $\Delta \tilde{T}(d)$ is computed by the FEM simulation.

2.5 Results

In this section the results of numerical simulations are discussed, ranging from the validity of such results to the analysis of the generated data. The former is mandatory to assert the veracity of the latter, as we don't have (yet) experimental data to verify the new results.

2.5.1 Validity of models

To validate a model, one needs to compare it to a ground truth while varying parameters to check its range of validity.

In our case, as we don't have experimental data to validate any claim, we have to rely on the assumption that the semi-analytical model converges to the correct solution given arbitrary high precision. In other words, if the model isn't subject to a change in its output while increasing the precision of a parameter (e.g. we increase W_x) while the other remain unchanged, this means that the parameter is precise enough.

Note that this is a iterative process as we need to check parameters one by one.

A priory, there's isn't any parameter which negatively impact the contribution of another. In other words, once a parameter is precise enough, changing another one should not result in the need to re-treat the previous one. This is under the assumption that at the start of this process, a good enough set of parameters as been chosen (i.e. no initial parameter value degrades the output dramatically).

Semi-analytical model

The semi-analytical model, as presented in [subsection 2.4.3](#), has already been validated by an experimental setup⁵. As it was only lightly modified (wrapping around existing code to pass run parameters more easily), there is no need to compare it to new experimental data to validate it.

However, it is useful to run convergence tests on simulation parameters (N_ξ , N_ζ , W_x and W_y) to verify that the program still works with our geometry.

⁵Private discussion with Bjorn Vermeersch about the simulation tool, 2024 IMEC

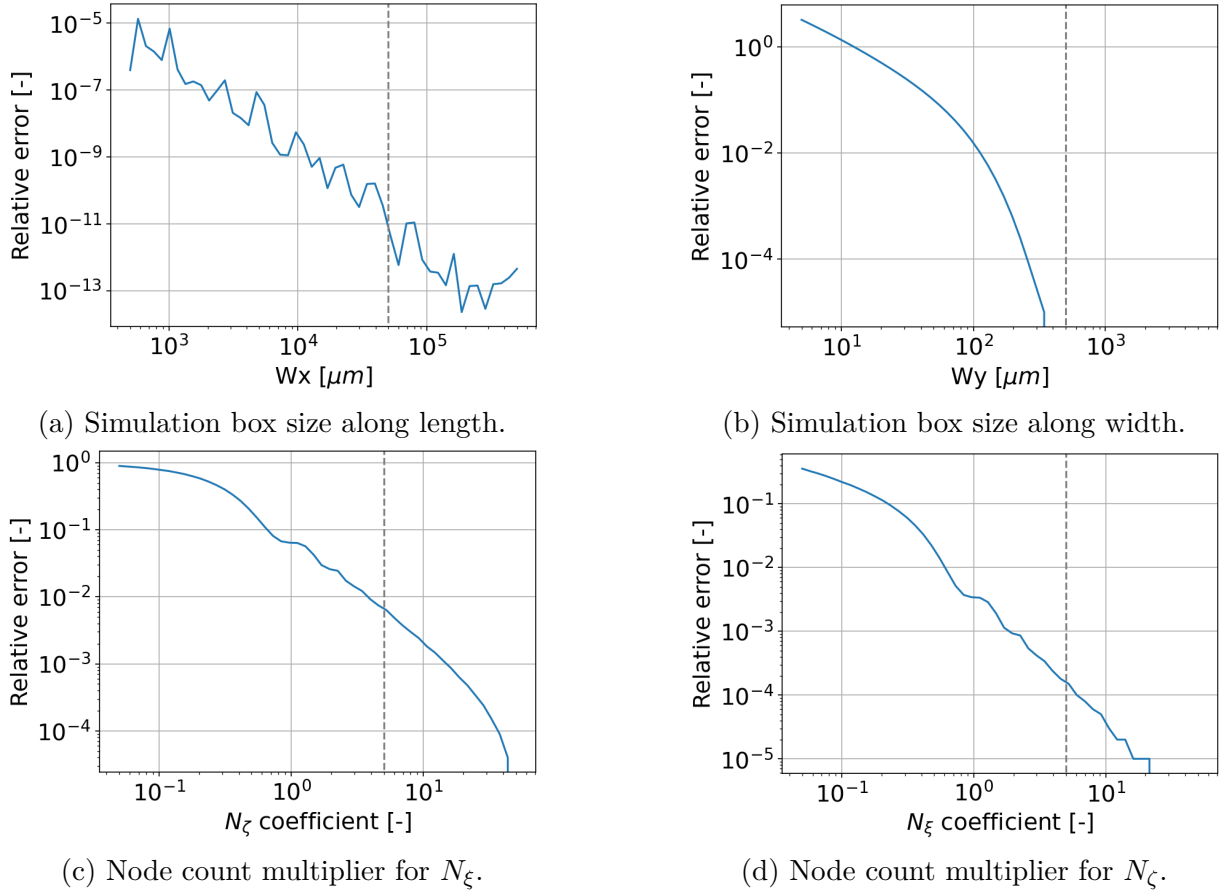


Figure 2.11: Convergence tests for various simulation parameters. The grey line indicates the nominal value of the parameter.

We define the relative error as:

$$e_f(k, s_{\text{nom}}) = \left| 1 - \frac{f(k, s_{\text{nom}})}{f(k_{\text{max}}, s_{\text{nom}})} \right|, \quad (2.35)$$

where k is the current parameter (sweep-ed), s_{nom} are the other parameters (fixed), k_{max} is value of k corresponding to the highest precision and $f(k, s_{\text{nom}})$ is the output value for a set of parameters. The evolution of this relative error is represented in Figure 2.11 for various parameters.

We see that for this choice of parameters, the error is always less than 1%. Also, to improve results while keeping a constant number of nodes (i.e. keeping the product $N_\xi N_\zeta$ constant), we could decrease the N_ζ coefficient from 5 to 2 and increase the N_ξ coefficient from 5 to 10.

However, we have to keep in mind that the parameters of interest for a run (i.e. those which will impact device performances) are the thickness of the different layers. Thus, we should expect the heat to spread more in certain cases, requiring higher values of W_x and W_y . The dimensions of the heat source won't be changed, so we can change the value of N_ξ and N_ζ without too much worry.

In the end, all parameters will be kept to their actual values.

FEM model

A similar analysis can be done with meshes for the FEM model.

However, we should expect more simulation artefacts when changing mesh parameters as the mesh is no longer structured. See **annex:GMSH** for an explanation of the meaning of the different mesh parameters.

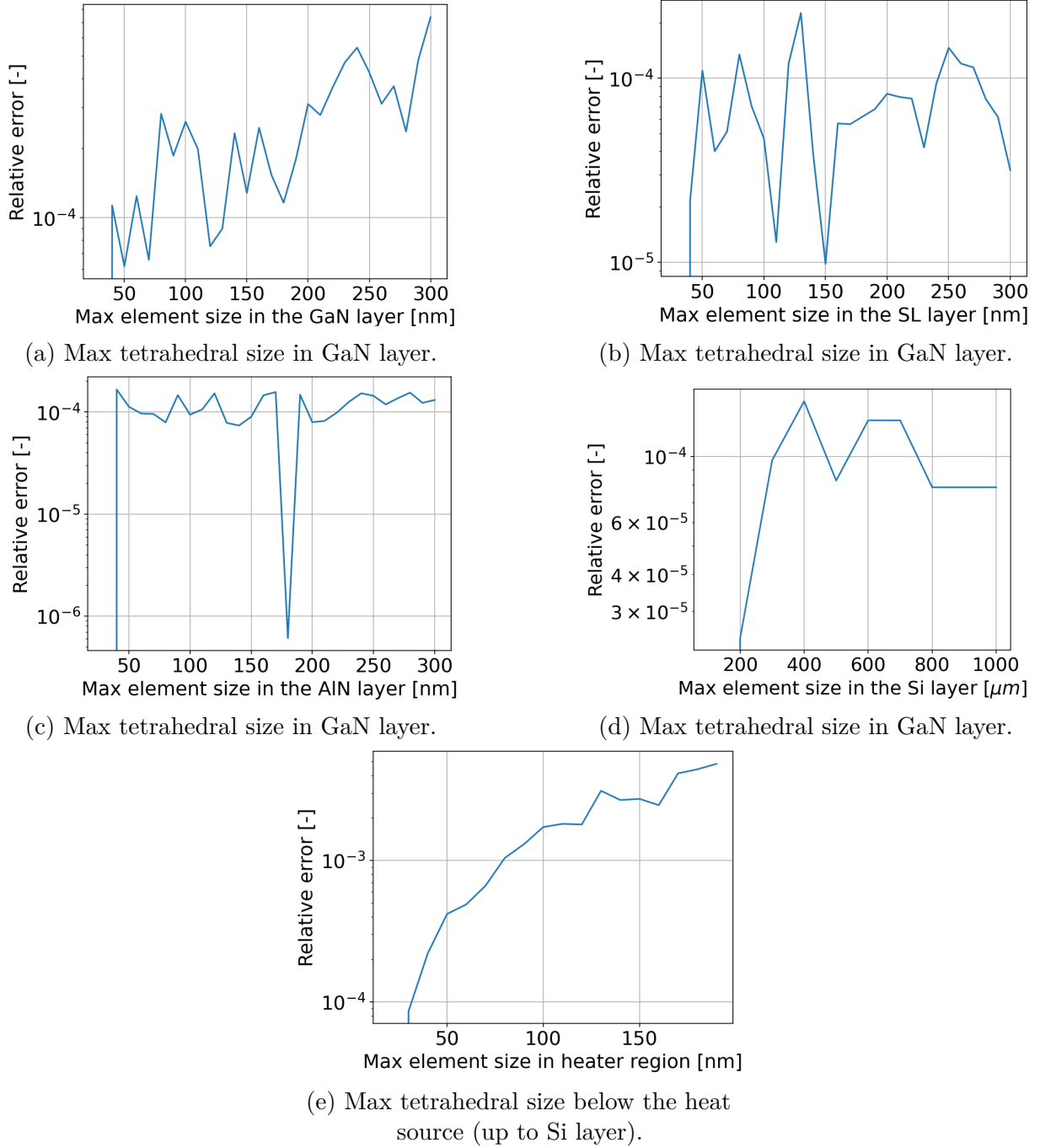


Figure 2.12: Convergence tests for various simulation parameters. The grey line indicates the nominal value of the parameter.

We can see in [Figure 2.12a](#) through [Figure 2.12d](#) that letting the elements grow bigger in size doesn't really impact the quality of the solution.

However, this doesn't mean that we could use elements several times bigger than a layer thickness. Even if let the elements grow as they want, they are always limited by two factors:

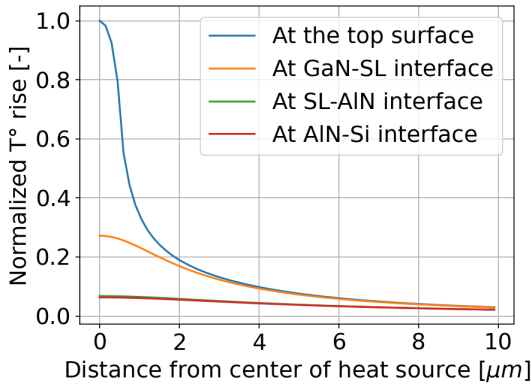
1. The size of the elements in the mesh is (approximately) continuous and can only grow so much over a short distance.
2. The elements are constrained in size in the cross-plane direction by the layer thickness.

This first point refers to the fact that we have a volume (or equivalently a surface in 2D) that is filled with elements which are connected by their faces and edges. In other words, a small element will share a side (in its case bigger than its order sides) with a big element. As the elements are not ill-shaped (i.e. they don't have a high aspect ratio between their sides), the change in size between two neighbor elements is limited.

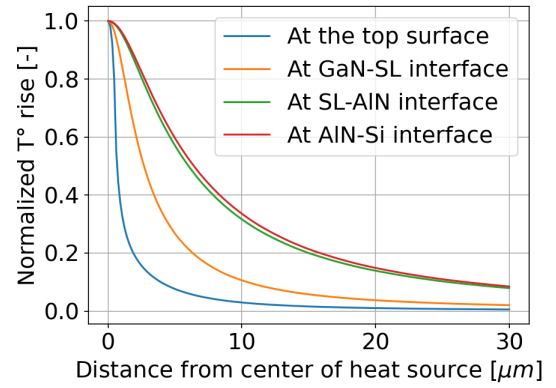
So the actual element size near the high resolution zone doesn't grow linearly (or at all above a certain threshold) with the maximum allowed.

The difference in the GaN layer case is that it is the first layer. The discontinuous nature of the heat source (perfect rectangle) will have most impact in those shallow depths as heat hasn't spread out yet. This spreading smooths the temperature profile in the in-plane direction the deeper we go into the device and thus a good precision is required here to avoid any issue.

This is akin to avalanche effect, in the sense that small perturbation in the GaN layer will amplify the farther it propagates from the heat source, in the cross-plane direction.



(a) Normalised with respect to $T_{\max}$.



(b) Normalised with respect to T at $y = 0$.

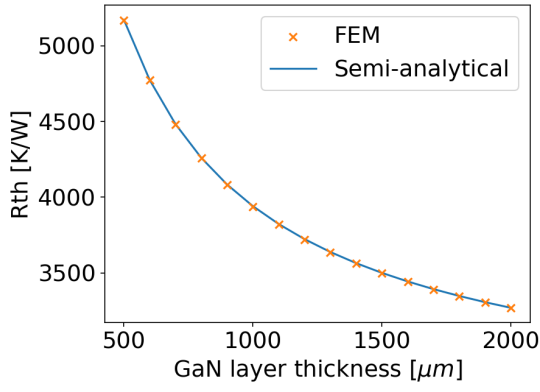
Figure 2.13: Example of the effect of heat spreading at different depths in the device along the y (width) direction. The 0 marks the center of the heat source.

While the temperature at the center decrease the deeper we go, as shown in Figure 2.13a, we can see that the temperature is more spread out as shown in Figure 2.13b. Note the difference in the scale of the x-axis between the two figures to make the effect of spreading more obvious.

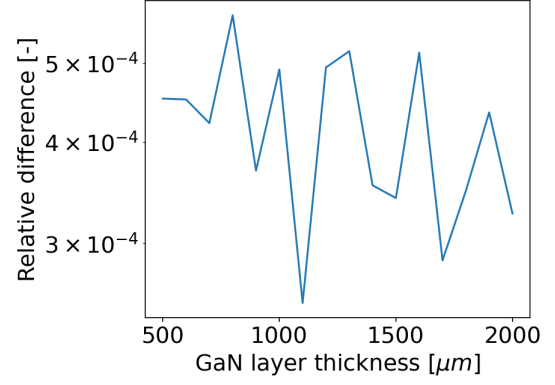
For the case of Figure 2.12e, this region underneath the heat source dictates the minimum size of the elements in the region where most of the heat is contained, i.e. where most of the details are. Thus it is important to have the greatest precision here, as confirmed by the convergence graphs.

Comparing semi-analytical with FEM

Now that each simulation has a correct set of parameters, we can try and compare them to see if there's divergence between them or not.



(a) Absolute values.



(b) Relative difference: $|1 - \frac{f_{FEM}(k)}{f_{TQM}(k)}|$.

Figure 2.14: Difference between semi-analytical model (TQM) and FEM for a $1\mu m \times 1\mu m$ heat source.

As shown in Figure 2.14, the results of both simulations agree with each other almost perfectly. The relative difference is less than 0.1% which is acceptable.

Taking the full Si thickness into account

As discussed before, the semi-analytical simulation is limited to a *thin* layer of Si (in this case $50\mu m$) compared to the full thickness of $\sim 1\text{mm}$. We have to validate this choice of Si layer thickness as to see whether it introduces too much edge effects or not.

Those edge effects come from the fact that the isothermal sink is different from the layer it is attached to. In other words, the effective in-plane thermal conductivity (it is effective for the heat sink as it doesn't have one per say) of the thermal heat sink is different than the one for the material just above. So much so that it is in fact infinite on this boundary as the temperature is constant on its entirety.

Thus, the heat flow should be perpendicular to the boundary so that there is no heat flowing in the in-plane directions.

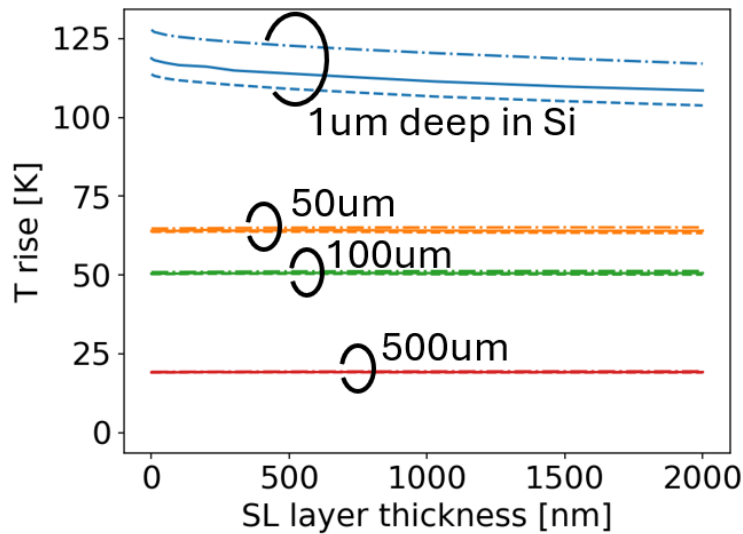


Figure 2.15: Temperature rise at different depths in Si (from AlN-Si interface) for different GaN layer thickness. The solid, dashed and dotted lines corresponds to $1.3\mu m$, $2\mu m$ and $0.5\mu m$ respectively.

As shown in Figure 2.15, the effects of the different GaN layer thickness on the temperature rise at $1\mu m$ from the AlN-Si interface are quite noticeable. However, the deeper we go into the Si layer, the less we notice those effects. This is due to the fact that most of the heat spreading happens in the 3 upper layer, where the device is located. The Si layer acts as a series thermal resistance which affects the dynamics of the device only as a shift in temperature.

This means that if we take into account enough Si, in this case $50\mu m$ seems to be acceptable, there shouldn't be any impact on the semi-analytical simulation.

2.5.2 Temperature rise

As the models have been validated, we can start simulating and analysing results.

We have 3 main parameters to play with: the thickness of the 3 top layers. The GaN layer has a base thickness of $1.3\mu m$, the SL layer has one of $1.03\mu m$ and the AlN layer $175nm$. Each of those layers has an anisotropic thermal conductivity (in-plane and cross-plane being different) which changes with layer thickness. The Si layer is different as it is thick enough to be considered bulk.

These information have seen summarized in the following figure ⁶.

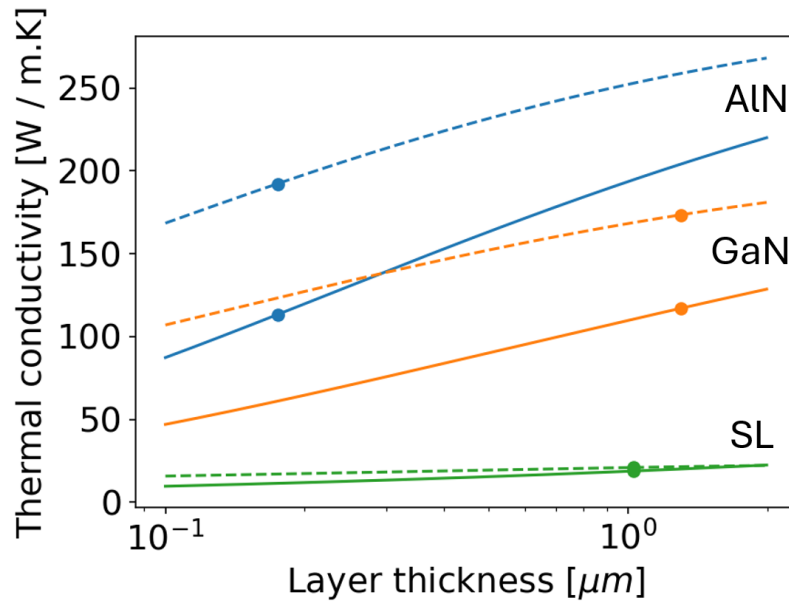


Figure 2.16: Thermal conductivity of different layers by layer thickness. The cross-plane thermal conductivity is shown in solid line and the in-plane one in dashed line. Dots show the base values.

	$\kappa_{\perp}$ [W/m.K]	$\kappa_{//}$ [W/m.K]
GaN	117	173
SL	19	21
AlN	113	192
Si	156	156

Table 2.1: Thermal conductivity of each layer at their base layer thickness.

⁶Those values come from BTE simulations done by Bjorn Vermeersch at IMEC.

Sensitivity to layer thickness (top surface)

Intuitively, the thicker the layer the higher the total thermal resistance will be. However, as show in Figure 2.16, the thermal conductivity goes up at the same time. So there's a competition between two effects which makes sensitivity of each layer thickness hard to guess without running the simulations.

We can define the dimensionless sensitivity $\tilde{S}_f^{(k)}(s^*)$ of a quantity f to a parameter k at a set of parameters s^* ($s^* = (k^*, \dots)$ being one of them) as follows:

$$\tilde{S}_f^{(k)}(s^*) = \left. \frac{\partial f}{\partial k} \right|_{s=s^*} \cdot \frac{k^*}{f(s^*)}. \quad (2.36)$$

The second part of this equation takes care of the normalisation. This normalisation ensures that we look at relative changes in both the monitored quantity and the current parameter of interest. In other words, by which factor is the output quantity multiplied (this sensitivity doesn't output that exact value but one which is closely related) when we multiply the parameter of interest.

The advantage of this approach, instead of just taking the derivative, is that we can compare parameters which are orders of magnitude different in the same manner. For example, it makes more sense to compare the effect of doubling of layer thicknesses for the GaN ($1.3\mu m$) and AlN layer ($0.175\mu m$), which is represented by the dimensionless sensitivity. However, if we just add $1\mu m$ of thickness to both layers, we should expect a more dramatic change in the AlN case as the layer thickness is multiplied by factor greater than 6.

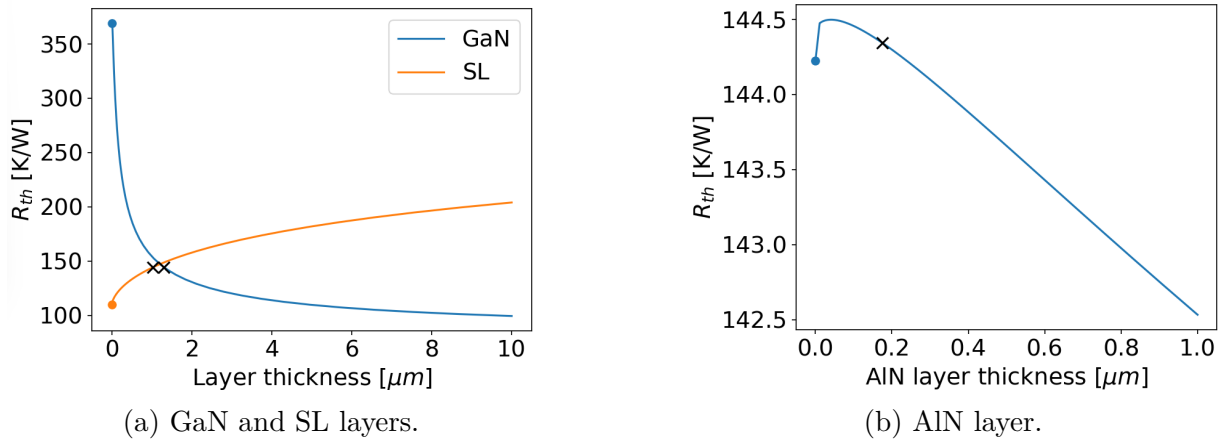


Figure 2.17: Thermal resistance of the system as a function of layer thickness. The dots show the value when the layer of interest is removed (thickness = 0). The crosses show the value for nominal layer thickness. Tests done for $50\mu m$ Si.

We can extract from graphs in Figure 2.17 the sensitivity for the different layers:

	GaN	SL	AlN
Sensitivity [-]	-0.31504	0.12994	-0.0006

Table 2.2: Dimensionless sensitivity of R_{th} to layer thickness around nominal parameters ($t_{GaN} = 1.3\mu m$, $t_{SL} = 1.03\mu m$ and $t_{AlN} = 175nm$).

Negative sensitivity implies a reduction in the temperature rise at the heat source (equivalent to the thermal resistivity of the system) as the layer thickness increases. This is consistent

with the graphs on [Figure 2.17](#) (sensitivity taken around the black crosses).

For the SL layer we see normal behaviour: the sensitivity of thermal resistivity of the whole system is positive. But for the GaN and AlN layers this is the opposite.

The explanation this phenomenon is that the in-plane thermal conductivity of both layers is superior to that of silicon. This results in a more efficient spreading of the heat in those layers compared to the bulk Si.

At the same time the thermal resistivity of the layer of interest increases but this change is compensated by the increase of thermal conductivity when increasing the layer thickness (as shown in [Figure 2.16](#)). This is however difficult to precisely quantify and of little interest.

Sensitivity to layer thickness (AlN-Si interface)

Now that the behaviour of the temperature rise at the top surface is understood, we have to model the one at the AlN-Si interface.

Little to no conclusion was made about the previous information because ultimately we are interested in what happens at the said interface. Knowing how the temperature in channel behaves is important as a number of material and electrical properties (e.g. carrier mobility) heavily depends on the local temperature.

This subject is far too complex to be briefly discussed and outside the scope of this master thesis. However, a good rule of thumb is that we want to be as close (or lower) to room temperature. This means we want the smallest temperature rise at the top surface.

The same can be said about the AlN-Si interface. But here the modelling is more complex as the temperature rise will be lower than at the top due to the layers acting as thermal resistors. This means that even if the thermal resistance of the whole system increases with a layer thickness, the temperature at the AlN-Si interface can decrease due to the increase of thermal resistance between the two surfaces.

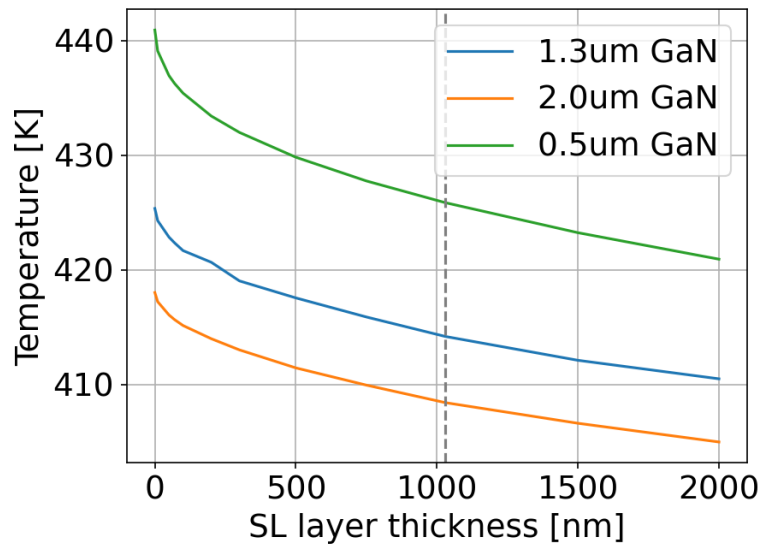


Figure 2.18: Example of (absolute) temperature at the AlN-Si interface. The gray dashed line indicates nominal SL layer thickness.

As shown in [Figure 2.18](#), we observe two different behaviours. The first is that the temperature at the AlN-Si interface decreases as the GaN layer thickness increases. This is consistent with what was discussed just before (for the top surface).

However, we also have a decrease in temperature as we increase the SL layer thickness, which would mean a negative sensitivity. This is due to the fact that the SL layer has a really poor conductivity (~ 10 times lower than bulk Si) which acts as a good thermal insulator and thus keeps the interface cool (low heat can pass through).

This is better shown in the following graph.

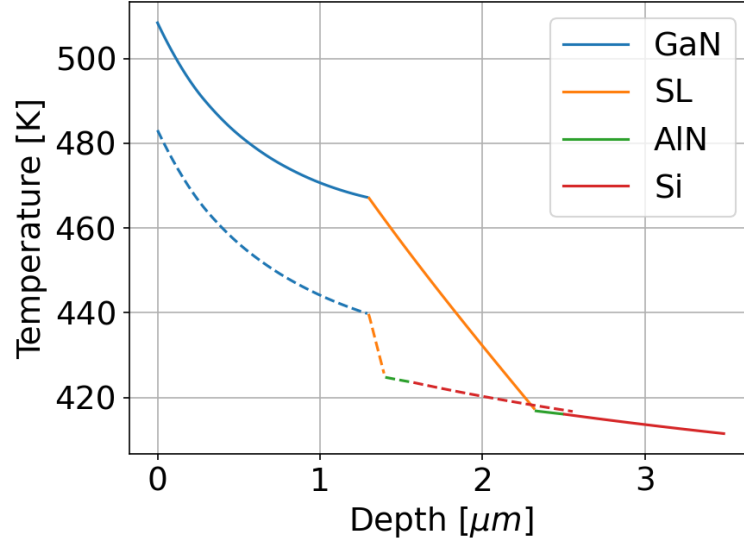


Figure 2.19: Temperature distribution near the heat source for nominal parameters (solid) or a SL layer thickness of 100nm (dashed). The different layers are highlighted.

We see on [Figure 2.19](#) that for a thinner SL layer we have a lower temperature at the surface (depth = 0) but at the same time the temperature at the AlN-Si interface is higher. Again, this is due to the poor conductivity of the SL layer which separate the two region from each other thermally.

Notice how the temperature distribution in the GaN layer is highly non-linear even though the layer is thin. This is due to the heat which is crammed in the tiny heat source being able to freely spread out.

AlN is similar to GaN in that sense it spreads heat well (better actually), but its impact is reduced due to the fact that it is situated underneath the SL layer, which is the main thermal bottle neck. Recalling the simple relationship [Equation 2.11](#) (which is only good as a insight in this case), the SL layer sees from one side the heat source widened by the GaN layer and the isothermal heat sink widened by the Si and AlN layer. However, the heat sink is infinitely wide (and large) so it is limited in effective size (as seen by the SL layer) by the layers in between. As the Si layer is more than 1000 times thicker than the AlN one, the latter has little to no influence, which explains the scale of the y-axis on [Figure 2.13b](#). On the contrary, the GaN layer is alone on its side of the thermal bottleneck, it has full influence on the effective size of the heat source as seen by the SL layer.

2.5.3 Resistivity and temperature

Now that the behaviour of the temperature distribution in the device with respect to the layer thicknesses is understood, we can apply it to a model of resistivity.

Resistivity model

Mobility in silicon is a very well known topic and is subject of most textbook on semiconductors. Its main parameters are the temperature of the material, its amount and type of doping. One such doping materials is Boron which is used for p-type doping.

An expression for mobility, not accounting interface effects which can become complicated pretty fast, is as follow [15]:

$$\mu_{tot}^{-1} = \mu_{th}^{-1} + \mu_{imp}^{-1} \quad (2.37)$$

$$\mu_{th} \propto T^{-3/2} \quad (2.38)$$

$$\mu_{imp} \propto T^{3/2}/N_{imp}, \quad (2.39)$$

where N_{imp} is the concentration of impurities (dopants). Equation 2.37 is Matthiessen's rule. The two other relations state that the contribution of the lattice to the mobility decreases with temperature. The impurity dependence however increases with temperature and decreases with their density.

Those temperature dependencies are a consequence that in this model the atoms have a limited sphere of influence and the electrons follow ballistic trajectory in between collision. Also, once they collide their velocity is given by the temperature of the system.

The inversely proportional relationship between mobility and concentration for the impurity related component of the mobility is due to the fact that the more impurities there is, the more chance an electron to collide with one, lowering on average the mobility.

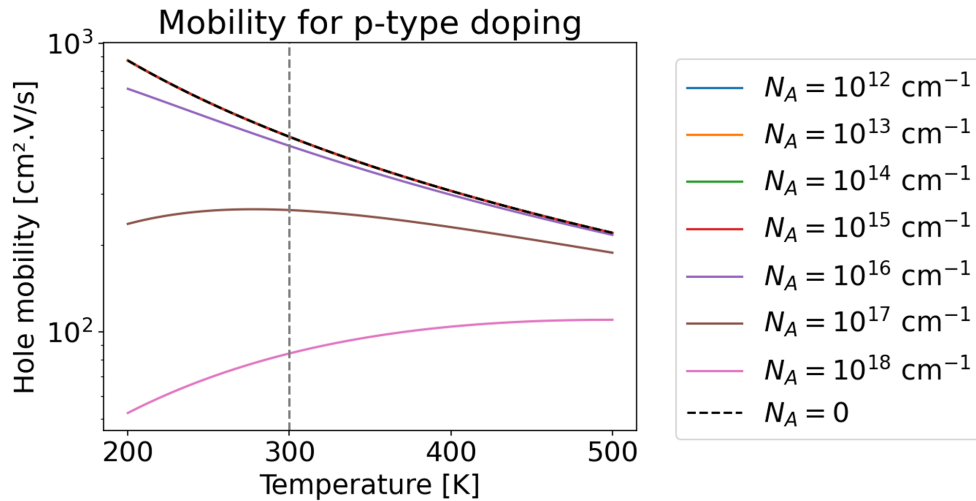


Figure 2.20: Mobility of holes in silicon for different impurity concentrations. This is for Boron doping (p-type).

As we can see in Figure 2.20, substrate with low doping (i.e. less than 10^{16} cm^{-3}) have a mobility dominated by the lattice contribution.

Now for the resistivity, we have formula which depends directly on the mobility and the carrier concentration:

$$\rho^{-1} = e(n\mu_n + p\mu_p), \quad (2.40)$$

where n refers to electrons (or their concentration) while p refers to hole (or their concentration). e is the charge of the electron.

The electron and hole concentrations are tied to electric charge neutrality: $N_d + p = N_a + e$. This means that in doped materials (e.g. $N_d \gg N_i$), the concentration of charges is equal to the dopant (e.g. $p = N_d$) while the minority carrier is negligible. However, when increasing the temperature, the intrinsic concentration of carrier increases:

$$n_i \propto e^{\frac{-E_g}{2k_b T}}, \quad (2.41)$$

where E_g is the band-gap energy and k_b is Boltzmann constant.

This increase make the minority carrier exceed the number of dopants leading to an increase of both carrier types.

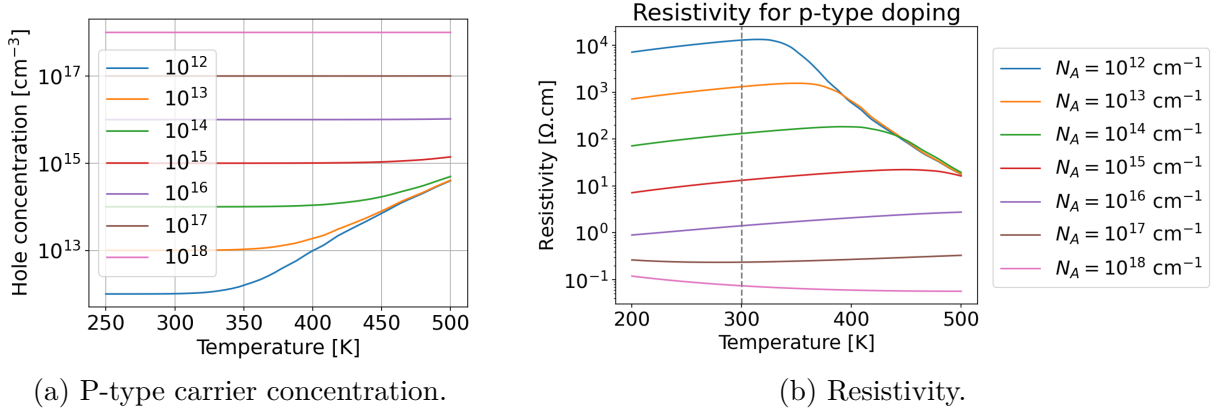


Figure 2.21: Temperature dependency of carrier concentration and resistivity for p-type doping (Boron) in silicon.

As we can see in [Figure 2.21a](#), the lightly doped substrate experience first the increase of n_i with temperature. This change comes from the fact that at those temperature $p = n = n_i$ as $n_i \gg N_d$ or $n_i \gg N_a$.

In [Figure 2.21b](#), we see that lower doped materials have higher resistivity. Also, we can clearly see the effect of increasing carrier density dropping the resistivity as they are inversely proportional.

Using resistivity model with temperature distribution

As discussed just before, increasing either (or both) SL or GaN layer thickness result in a decrease in temperature at the AlN-Si interface. Combined with the resistivity decreasing with temperature, we get that resistivity increases with layer thicknesses, as represented in the upper-right corner of [Figure 2.22](#).

Unfortunately, even in good conditions (room temperature heat sink), the drop in resistivity is quite high. In this case, even though this is a HR substrate ($\sim 7.5k\Omega.cm$ at room temperature), the resistivity goes to only a couple hundred $\Omega.cm$.

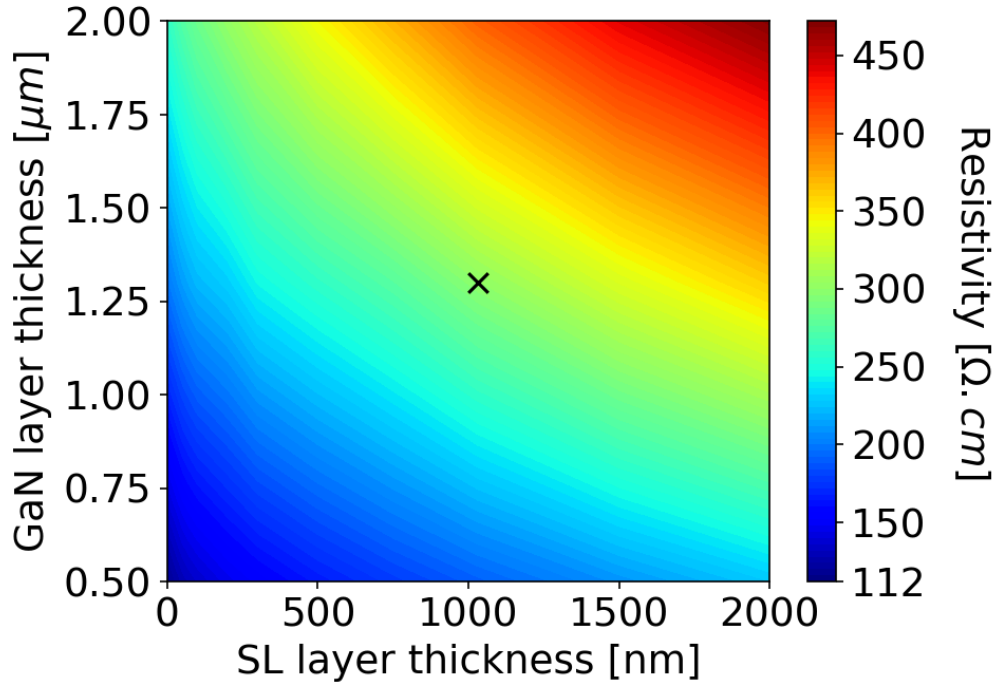


Figure 2.22: Resistivity at the AlN-Si interface for varying layer thicknesses. The temperature of the heat sink is set to 300K. The cross indicates nominal parameters.

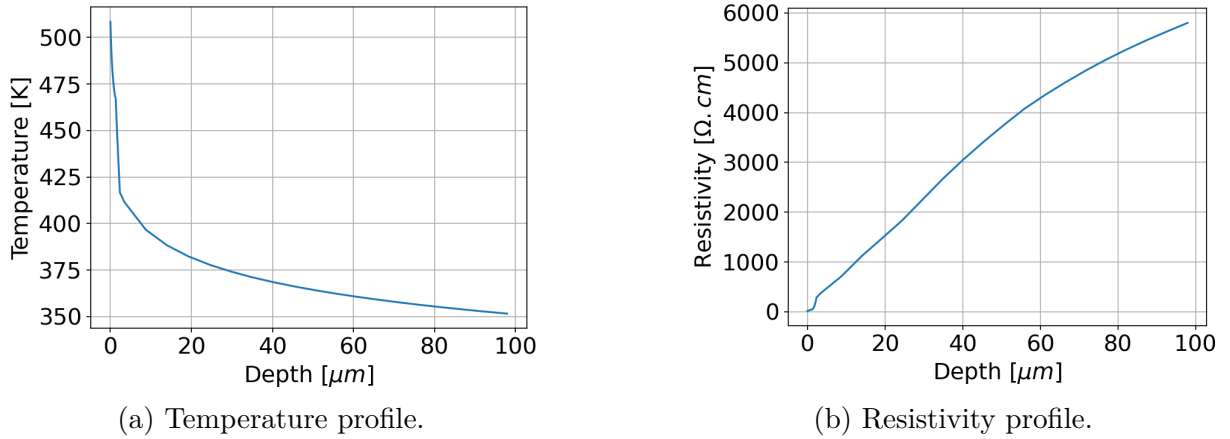


Figure 2.23: Temperature and resistivity profile in the device with nominal parameters. This shows only the first $100\mu m$ of the total thickness.

As shown in [Figure 2.23b](#), the resistivity quickly increases to a few thousand of $\Omega.cm$ in a matter of tens of micrometers. This fact reflects the exponential nature of the drop in resistivity.

Also, as shown in [Figure 2.23a](#), about half of the temperature drop occurs before the Si layer. Reducing the Si layer thickness could improve the results dramatically, to the point of suppressing it almost completely (again, if the heat sink is perfectly cooled to 300K) as shown in the next figure.

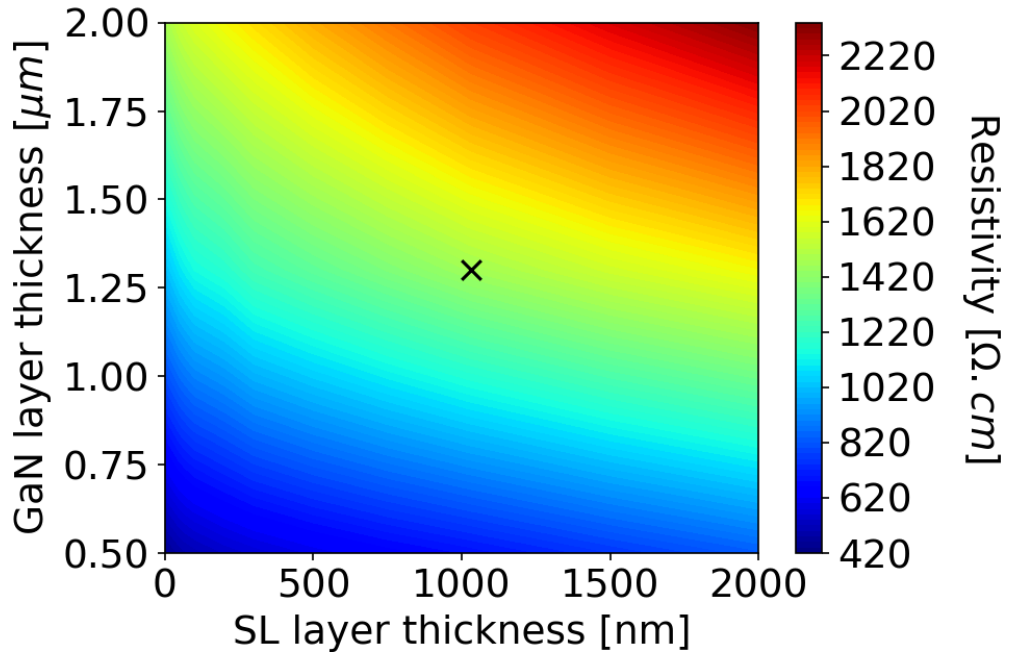


Figure 2.24: Resistivity at the AlN-Si interface for varying layer thicknesses. The temperature of the heat sink is set to 300K and there is only $50\mu m$ of Si. The cross indicates nominal parameters.

Chapter 3

3-omega technique

3.1 Theoretical considerations

3.1.1 Simple analytical model of voltage

The physical principle behind the 3ω technique is the linear approximation of electrical resistance as a function of temperature. Indeed, we can model a resistor at the first order as:

$$R_h(T) = R_{h,0}(1 + \beta_h \Delta T), \quad (3.1)$$

where $R_{h,0}$ is the value of the electrical resistance at a reference temperature T_0 (such that $T = T_0 + \Delta T$) and β_h is the Temperature Coefficient of Resistance (TCR) of the resistor. This TCR is usually on the order of $10^{-3} [\text{K}^{-1}]$.

Now, if we pass a current $I_{1\omega}(t)$ oscillating around a fundamental radial frequency ω

$$I_{1\omega}(t) = I_0 \cos(\omega t) \quad (3.2)$$

into the resistor, we observe, according to Ohm's law, a resulting voltage $V_{1\omega} = R_h I_{1\omega} = R_h I_0 \cos(\omega t)$. This current will also produce a Joule heating in the resistor:

$$P(t) = R_h I_{1\omega}^2 = R_h I_0^2 \frac{1 + \cos(2\omega t)}{2}. \quad (3.3)$$

This heat will interact with the environment, dissipating where it can, and raising the temperature accordingly. This results in a change of temperature, proportional to the given heating power, in the heater. This temperature rise ΔT can be written as:

$$T = T_0 + \Delta T \quad (3.4)$$

$$\Delta T = \Delta T_{DC} + \Delta T_{AC} \cos(2\omega t + \phi) \quad (3.5)$$

If we put [Equation 3.5](#) into [Equation 3.1](#) and multiply by the input current $I_{1\omega}$, we get a voltage across the resistor:

$$V(t) = \underbrace{R_{h,0}(1 + \beta_h(\Delta T_{DC} + |\Delta T_{AC}| \cos(2\omega t + \phi)))}_{R_h(t) = R_{h,DC} + R_{h,AC}(t)} \underbrace{I_0 \cos(\omega t)}_{I_{1\omega}(t)} \quad (3.6)$$

Using the relation $\cos(a) \cos(b) = \frac{\cos(a+b) + \cos(a-b)}{2}$, we can re-write the output voltage as:

$$\begin{aligned} V(t) = & I_0 R_{h,0} (1 + \beta_h \Delta T_{DC}) \cos(\omega t) \\ & + I_0 R_{h,0} \beta_h |\Delta T_{AC}| \frac{\cos(\omega t + \phi) + \cos(3\omega t + \phi)}{2} \end{aligned} \quad (3.7)$$

Isolating each term in Equation 3.7 leads to the following table:

Frequency	Phase-shift	Voltage
ω	0	$I_0 R_{h,0} (1 + \beta_h \Delta T_{DC})$
ω	ϕ	$I_0 R_{h,0} \beta_h \Delta T_{AC} /2$
3ω	ϕ	$I_0 R_{h,0} \beta_h \Delta T_{AC} /2$

Table 3.1: Decomposition of voltages in terms of angular frequency and phase-shift compared to input current $I_{1\omega}(t)$

According to Euler's formula ($e^{j\phi} = \cos(\phi) + j \sin(\phi)$ with j the imaginary unit), we can split the 3ω component in a in-phase component (real part) and out of phase component (imaginary part):

$$V_{3\omega,i} = I_0 R_{h,0} \beta_h |\Delta T_{AC}| \cos(\phi)/2 \quad (3.8)$$

$$V_{3\omega,o} = I_0 R_{h,0} \beta_h |\Delta T_{AC}| \sin(\phi)/2 \quad (3.9)$$

$$V_{3\omega} = V_{3\omega,i} + jV_{3\omega,o} \quad (3.10)$$

This whole procedure is resumed in the following diagram:

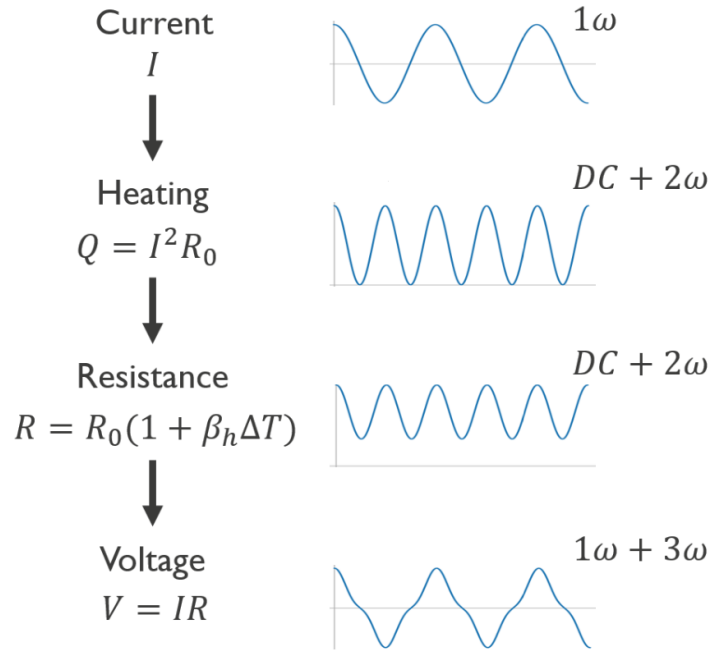


Figure 3.1: Signals in the 3ω technique. Inspired by (p17 of Ch2 of Dames).

3.1.2 Heat propagation in a (semi) cylinder

We are interested in the behaviour of the thermal oscillations in the material as a function of frequency and the geometry of the device under test below the heater. One useful approximation (which further discussed later) is that the heater is infinitely long. In other words, the heats spread radially in the cross-plane direction and only one of the in-plane directions.

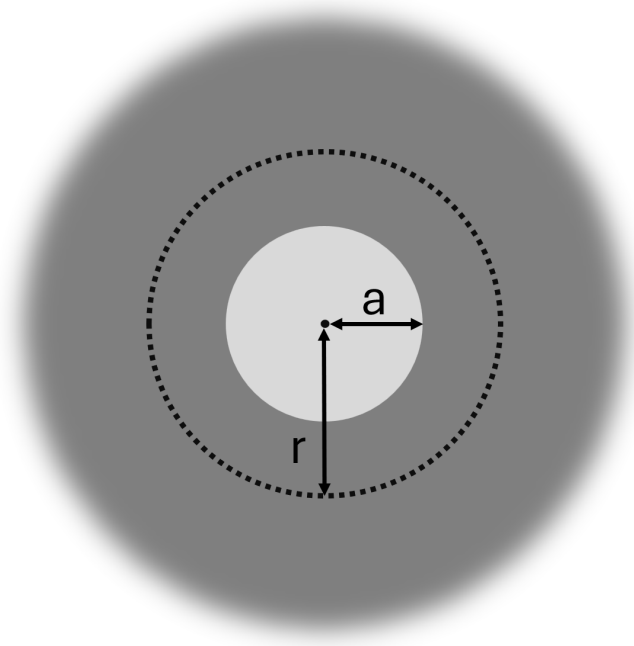


Figure 3.2: Schematic of a 1D cylindrical heater of radius a (light gray) in an infinite homogeneous substrate (dark gray).

This is akin to a 1D cylindrical heater as shown in [Figure 3.2](#). The governing heat equation in steady-state can be written in the cylindrical coordinate system:

$$\frac{\partial^2 \Delta T_{AC}(r, t)}{\partial r^2} + \frac{1}{r} \frac{\partial \Delta T_{AC}(r, t)}{\partial r} - \frac{1}{\alpha} \frac{\partial \Delta T_{AC}(r, t)}{\partial t} = 0, \quad (3.11)$$

where α is the diffusivity of the substrate.

Since those thermal oscillations are in steady-state, we can use the method of separation of variables to solve this problem:

$$\Delta T_{AC}(r, t) = |\Delta T_{AC}(r)| \cdot \Theta(t). \quad (3.12)$$

$|\Delta T_{AC}|(r)$ is what we're after, the radial evolution of the (frequency dependant) amplitude of the temperature oscillations, and $\Theta(t)$ the spatial evolution. The fact that $|\Delta T_{AC}|$ depends on ω (and not t) is not obvious but will become clear in a short while.

From [Equation 3.5](#), we know that the thermal amplitude oscillate at a frequency of 2ω . So we can write:

$$\Theta(t) = \cos(2\omega t) = \mathcal{R}\{e^{j2\omega t}\}, \quad (3.13)$$

where $\mathcal{R}\{.\}$ takes the real part of a quantity. Using this notation, we can re-write [Equation 3.11](#) as follows:

$$\mathcal{R}\left\{\frac{d^2 |\Delta T_{AC}|(r)}{dr^2} + \frac{1}{r} \frac{d |\Delta T_{AC}|(r)}{dr} - q^2 |\Delta T_{AC}|(r)\right\} = 0, \quad (3.14)$$

where q is the wave-number of the thermal wave, which is defined as:

$$q = \sqrt{j2\omega/\alpha}. \quad (3.15)$$

Where $\alpha = \kappa/\rho c_p$ is the diffusivity, ρ the density and c_p the specific heat capacity. This wave-number is better understood if we take its norm, which correspond to the thermal penetration wave-length:

$$\lambda = \frac{1}{|q|} = \sqrt{\frac{\alpha}{2\omega}}. \quad (3.16)$$

This quantity will be very important for all subsequent discussion as it gives us (approximately) the maximum depth at which a thermal wave can reach in a material. In other words, it gives an insight at how much of the system is the heater capable to see. This is one of the core strength of the 3-omega technique as this will allow us to see substrate (from the point of view of the heater) as semi-infinite or only certain layers selectively.

Coming back to Equation 3.14, it has taken the form of a modified Bessel equation of order 0 of the second kind, which has known solutions.

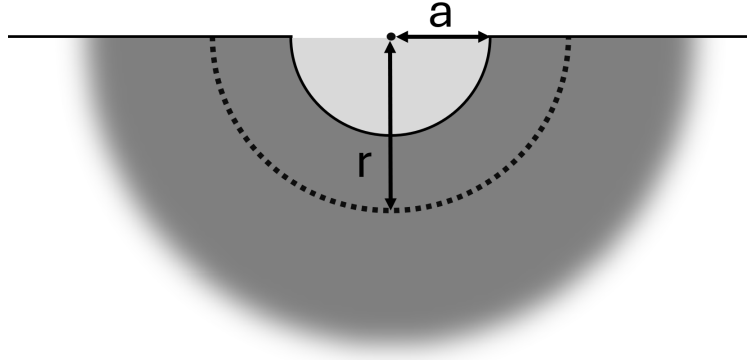


Figure 3.3: Schematic of a 1D cylindrical heater of radius a (light gray) in a semi-infinite homogeneous substrate (dark gray).

As the heat can only propagate in half the plane, the solution is only slightly modified: we just have twice the amplitude of the thermal oscillations. This leads to the following solution:

$$|\Delta T_{AC,i}|(r, \omega) = \frac{p_{rms}}{\pi \kappa} \mathcal{R}\{K_0(qr)\} \quad (3.17)$$

$$|\Delta T_{AC,o}|(r, \omega) = \frac{p_{rms}}{\pi \kappa} \mathcal{I}\{K_0(qr)\}, \quad (3.18)$$

where K_0 is a zero order modified Bessel function of the second kind and p_{rms} is the root mean square power supplied per unit heater length in [W/m]:

$$p_{rms} = \frac{R_{h,0} I_0^2}{2l_h}. \quad (3.19)$$

Note that we could equivalently define it using the voltage across the heater $V_{h,0} = I_0 R_0$:

$$p_{rms} = \frac{V_{h,0}^2}{2l_h R_{h,0}}. \quad (3.20)$$

Equation 3.17 and Equation 3.18 tell us that the thermal oscillations are highly localised, especially as their frequency increases.

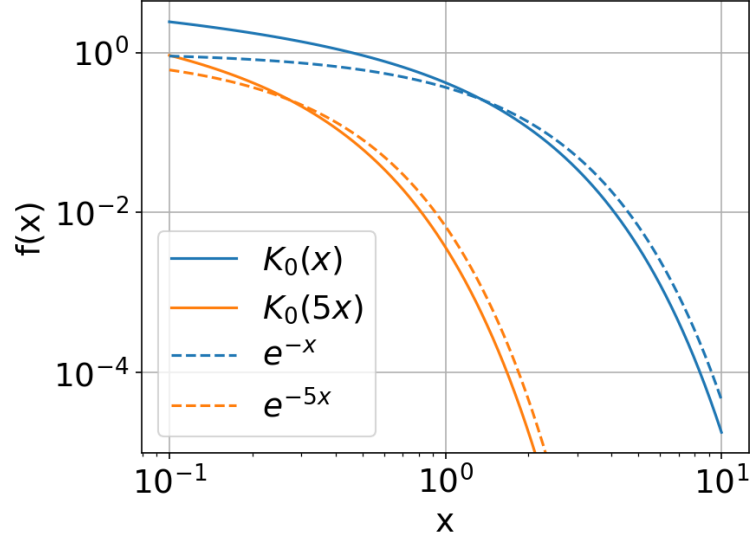


Figure 3.4: Comparison between $K_0(x)$ and e^{-x} which is known to decrease fast.

As show in Figure 3.4 the amplitude of K_0 decreases faster than exponentially, which means that the amplitude of the thermal oscillations decays rapidly as we get away from the heater.

It would be useful to define a rule of thumb to quantify this decrease in amplitude. Empirically, the amplitude of an exponential functions is reduced to less than 1% of its magnitude after 5 length constants. As K_0 is initially decreasing only slightly faster than the exponential, one should expect this same upper-bound for the 1% threshold. In other words, $\frac{K_0(0)}{K_0(5\lambda)} < 1\%$ for $r > 5\lambda$ which means that a layer with a thickness of more than 5λ can be considered as semi-infinite.

3.1.3 Finite width of the heater

Equation 3.17 and Equation 3.18 are defined for a one-dimensional heat source, but in reality it is a 3D object (a rectangular prism). The heat dissipation through radiation via the faces in contact with air can be neglected for now, shifting the modelling of the heat source to a 2D rectangle, which is still one dimension more than the previously discussed case.

However, this a simple problem which can be solved by using the Fourier transform along the width of the heater [16]. To take into account this width, we can simply take the convolution of the 1D solution with the heat distribution. This operation is just a multiplication in the Fourier domain, hence all the development done just before.

The euclidean distance of a point in the specimen from the origin can be simplified to $r = \sqrt{x^2 + y^2} = |x|$ as we're only interested in what happens at the surface of the heater ($y = 0$). This leads to the following formula for the of amplitude of thermal oscillations:

$$|\Delta T_{AC}|(\eta) = \int_{-\infty}^{\infty} |\Delta T_{AC}|(x) \exp(-j\eta x) dx \quad (3.21)$$

$$|\Delta T_{AC}|(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} |\Delta T_{AC}|(\eta) \exp(j\eta x) d\eta. \quad (3.22)$$

Equation 3.22 is simply the inverse Fourier transform of $|\Delta T_{AC}|(\eta)$.

η is the wave-number associated with the x coordinate. As the heater is symmetric with the origin, $|\Delta T_{AC}|(x)$ is expected to be even in x leading to simpler integrals:

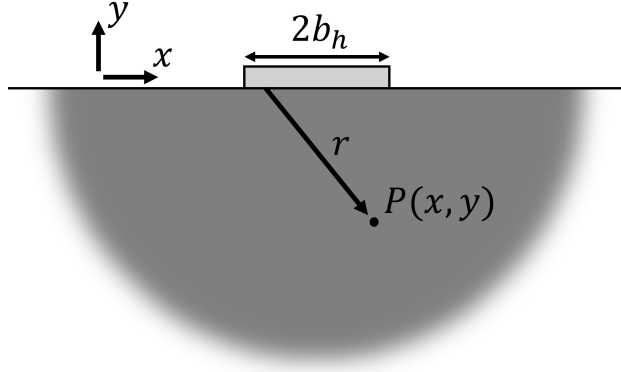


Figure 3.5: Schematic of a finite width ($2b_h$) heater with a single contribution from the heater to a point in the specimen.

$$|\Delta T_{AC}|(\eta) = 2 \int_0^\infty |\Delta T_{AC}|(x) \cos(j\eta x) dx \quad (3.23)$$

$$|\Delta T_{AC}|(x) = \frac{1}{\pi} \int_0^\infty |\Delta T_{AC}|(\eta) \cos(\eta x) d\eta. \quad (3.24)$$

This leads the temperature oscillations in the Fourier space to take the form:

$$|\Delta T_{AC}|(\eta) = \frac{p_{rms}}{2\kappa} \left(\frac{1}{\sqrt{\eta^2 + q^2}} \right). \quad (3.25)$$

By taking the assumption that the heat is uniformly dissipated in the heater, we can express is as a window function with a support of $|x| \leq b_h$. Its Fourier transform is given by:

$$\int_0^{b_h} \mathbb{1}_{[-b_h, b_h]}(x) \cos(\eta x) dx = \frac{\sin(\eta b_h)}{\eta b_h}. \quad (3.26)$$

To take into account this width, we can simply take the convolution of the 1D solution with the heat distribution. This operation is just a multiplication in the Fourier domain, hence all the derivations done just before.

Multiplying [Equation 3.25](#) with [Equation 3.26](#) we get:

$$|\Delta T_{AC}|(\eta) = \frac{p_{rms}}{\kappa} \left(\frac{\sin(\eta b_h)}{\eta b_h \sqrt{\eta^2 + q^2}} \right). \quad (3.27)$$

The measured temperature oscillation is the average value over the full width of the heater. Taking the inverse Fourier transform of [Equation 3.27](#) and integrating it over the heater we get:

$$|\Delta T_{AC}| = \frac{1}{b} \int_0^{b_h} \frac{1}{\pi} \int_0^\infty \frac{p_{rms}}{\kappa} \left(\frac{\sin(\eta b_h)}{\eta b_h \sqrt{\eta^2 + q^2}} \right) \cos(\eta x) d\eta dx \quad (3.28)$$

$$= \frac{p_{rms}}{\pi \kappa} \int_0^\infty \frac{\sin^2(\eta b_h)}{(\eta b_h)^2 \sqrt{\eta^2 + q^2}} d\eta. \quad (3.29)$$

This last result ([Equation 3.29](#)) will be referred to as Cahill's formula.

3.1.4 Approximate solutions to Cahill's formula

Equation 3.29 can be numerically integrated using common integration techniques to give us some insights in the shape of the solution. In the case of Figure 3.6, Python with Scipy's Simpson integration was used.

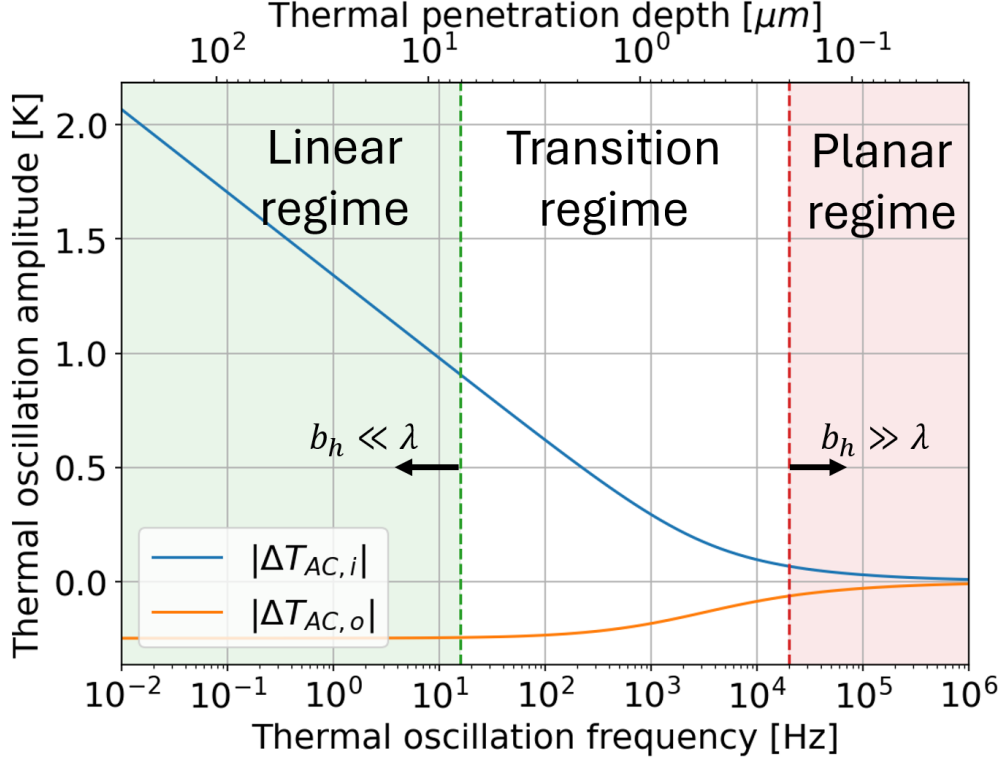


Figure 3.6: Cahill's formula numerically integrated via Simpson integration. The parameters are: a thermal conductivity $k = 1$ [W/m.K], a thermal diffusivity $\alpha = 100[\mu\text{m}^2/\text{s}]$, a heater half-width $b_h = 1[\mu\text{m}]$ and a rms dissipated heat power $p_{rms} = 1$ [W/m]. The three regimes have been highlighted.

As we can see, three distinct regimes appear:

1. The linear regime (large thermal penetration depths) where the in-phase component decreases logarithmically with frequency (linear with $\log(\omega)$) and the out-of-phase component is constant and negative.
2. The planar regime (small thermal penetration depths) where the in-phase and out-of-phase components are equal and opposite.
3. The transition regime where the behaviour of both components is way more complicated. It is a *transition* region where they switch from one of the previous regime to the other.

Linear regime

This regime is characterised by a large thermal penetration depth, with can be mathematically written as $\lambda \gg b_h$. We can write this condition as $b_h \rightarrow 0$ such that:

$$\lim_{b_h \rightarrow 0} \frac{\sin(b_h \eta)}{b_h \eta} = 1. \quad (3.30)$$

Also, due to the rapid decay of large wave-number oscillations and their relatively small amplitude, the integral in Equation 3.29 is dominated by wave-numbers in the interval $\eta \in [\frac{1}{\lambda}; \frac{1}{b_h}]$. Combining Equation 3.29 with Equation 3.30, we get:

$$|\Delta T_{AC}| = \frac{p_{rms}}{\pi\kappa} \int_0^{1/b_h} \frac{1}{\sqrt{\eta^2 + q^2}} d\eta \approx \frac{p_{rms}}{\pi\kappa} (\ln(qb_h) - \epsilon), \quad (3.31)$$

with ϵ being a fitting constant of approximately 0.923 ($= \frac{3}{2} - \gamma$, γ being Euler's constant) [17].

By expanding $q = \sqrt{\frac{j2\omega}{\alpha}}$ in Equation 3.31, we have the explicit dependency of the thermal oscillations $|\Delta T_{AC}|$ in terms of the excitation frequency 2ω :

$$|\Delta T_{AC}| = \underbrace{-\frac{p_{rms}}{2\pi\kappa} \left(\ln\left(\frac{b_h^2}{\alpha}\right) + \ln(2\omega) - 2\epsilon \right)}_{\text{In-phase}} - j \underbrace{\frac{p_{rms}}{4\kappa}}_{\text{Out-of-phase}}. \quad (3.32)$$

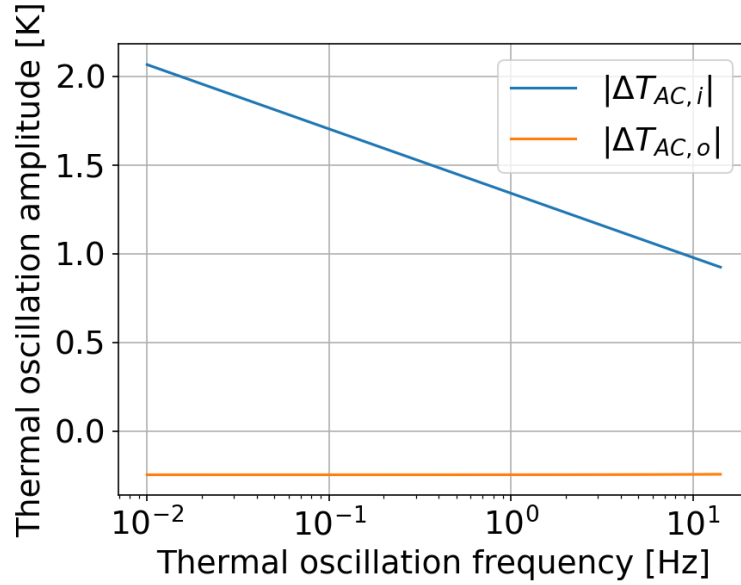


Figure 3.7: Amplitude of thermal oscillations (separated by components) as a function of frequency in the linear regime. The parameters are the same as in Figure 3.6.

As mentioned before, the amplitude of the in-phase component of the amplitude of the thermal oscillations is linear with respect to the logarithm of frequency, which is shown in Figure 3.7.

Combining Equation 3.10 with the new found Equation 3.32 we have model for the measured 3ω voltage:

$$V_{3\omega} = -\frac{V_0^3 \beta_h}{4\pi l \kappa R_0} \left(\ln\left(\frac{b_h^2}{\alpha}\right) + \ln(2\omega) - 2\epsilon \right) - j \frac{V_0^3 \beta_h}{8\pi l \kappa R_0}. \quad (3.33)$$

Moreover, we can see that the thermal conductivity appears explicitly in Equation 3.32 as a function of $\ln(2\omega)$.

We can take its derivative by this last quantity to get:

$$\frac{\partial |\Delta T_{AC}|}{\partial \ln(2\omega)} = -\frac{p_{rms}}{2\pi\kappa} \quad (3.34)$$

Combing Equation 3.33 with Equation 3.34, we have an experimental way to measure thermal conductivity from 3ω measurement:

$$\kappa = \frac{V_0^3 \beta_h}{4\pi l \kappa R_0} \cdot \frac{1}{\partial |\Delta T_{AC}| / \partial \ln(2\omega)}. \quad (3.35)$$

We could also extract the thermal conductivity from the out-of-phase component. However this approach was found to be less accurate in practice than the slope of the in-phase component [16].

Planar regime

This regime is characterised by a small thermal penetration depth, with can be mathematically written as $\lambda \ll b_h$. We can write this condition as $b_h \rightarrow \infty$ such that:

$$\lim_{b_h \rightarrow \infty} \frac{1}{\pi b_h} \left(\frac{\sin(\eta b_h)}{\sin(\eta)} \right)^2 = \delta(\eta). \quad (3.36)$$

Combining Equation 3.29 with Equation 3.36, we get:

$$|\Delta T_{AC}| = \frac{p_{rms}}{b_h \kappa} \int_0^\infty \frac{\sin^2(\eta)}{\eta^2 \sqrt{\eta^2 + q^2}} d\eta = \frac{p_{rms}}{2b_h \kappa q}. \quad (3.37)$$

Note that $\sqrt{q^2} \neq |q|$ due to the fact that q is a complex number. Using its definition (Equation 3.15), we have:

$$|\Delta T_{AC}| = \frac{p_{rms}}{2b_h \kappa \sqrt{2\omega/\alpha}} e^{-i\frac{\pi}{4}}. \quad (3.38)$$

In other words, the in-phase and out-of-phase components have the same value with opposing signs as mentioned before. This behaviour can be better seen in Figure 3.8.

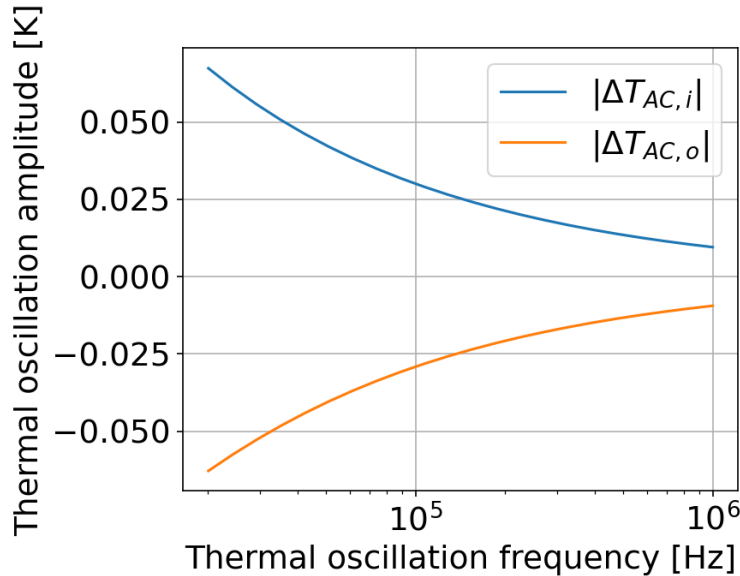


Figure 3.8: Amplitude of thermal oscillations (separated by components) as a function of frequency in the planar regime. The parameters are the same as in Figure 3.6.

This time, we can combine Equation 3.10 with Equation 3.38 to get a model for the measured 3ω voltage:

$$V_{3\omega} = \frac{V_0^3 \beta_h}{\sqrt{32} l b_h \kappa R_0 \sqrt{2\omega/\alpha}} (1 - j), \quad (3.39)$$

which can be re-written, to have another experimental way to measure thermal conductivity from 3ω measurement, as:

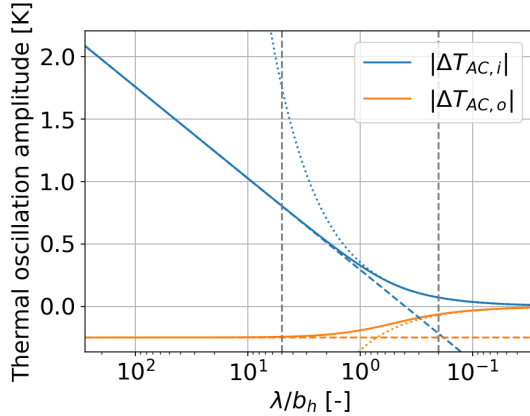
$$\kappa = \frac{V_0^3 \beta_h}{\sqrt{32} l b_h V_{3\omega} R_0 \sqrt{2\omega/\alpha}} (1 - j). \quad (3.40)$$

Equation 3.40 is however less suited to extract the thermal conductivity than Equation 3.35 as the amplitude of the 3rd harmonic of the electrical oscillations is way lower in the former case. This is due to the $1/\sqrt{\omega}$ factor which is really small in this regime of high thermal excitation frequency.

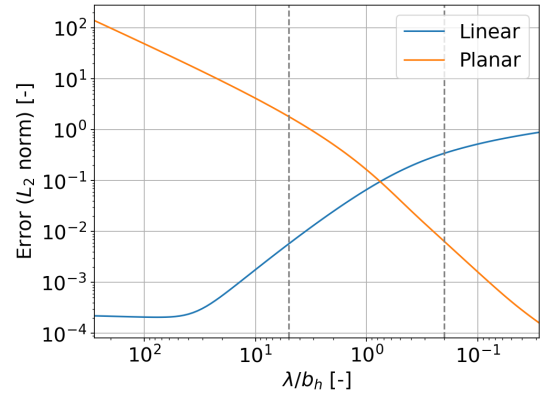
Nonetheless, this latter method gives us an additional way to characterise thermal diffusivity for a surface layer, as in this regime the thermal penetration depth is pretty small.

Approximation of both regimes

Now that we have approximations for both regime, we should take a how their error varies with the actual solution. This is useful to better quantify the validity of the bounds of the different regimes.



(a) Approximations. The solid, dashed and dotted lines correspond to Cahill's formula, the linear approximation and the planar approximation respectively.



(b) L_2 norm of the difference between Cahill's formula and the linear or planar approximation. This norm takes into account both components of each formula.

Figure 3.9: Difference between Cahill's formula and approximations as a function of the ratio of the thermal penetration depth and the heater half-width (same parameters as in Figure 3.6). Gray lines indicates λ/b_h of 0.2 and 5, being the limits of the planar and linear regime respectively.

As seen in Figure 3.9a, the approximations correspond well to exact solution within their corresponding regime. This is especially true for the in-phase component for which the bounds could be relaxed.

However, the total error, the magnitude of the difference between Cahill's formula and an

approximation (referred as the L_2 norm of the error), is a bit bigger. As shown in [Figure 3.9b](#), the approximation errors are just under the 1% threshold at the boundaries of the regimes ($\lambda/b_h = .2$ or 5). This confirms the validity of the value of those bounds.

3.1.5 Thin film and multi-layered system

The approximations derived until now make good prediction of the theoretical formula under the correct assumptions. This model was developed for an uniform specimen, in other words a relatively thick mono-layer. Efforts were made to render it semi-infinite from the point of view of the heater, limiting the possible non-idealities stemming from interactions between the thermal oscillations and the heat sink.

However, specimens of interest, especially in the scope of this master thesis, may be constituted instead of multiple layers on top of each other. This configuration is unfortunately outside the range of application of Cahill's formula in its current form ([Equation 3.29](#)). It needs to be modified in order to take into account those additional layers.

Thin film

It was proposed by Cahill [\[18\]](#) that in the case for 1D heat flow in thin film, there is an additional shift to the in-phase component in the linear regime:

$$\Delta T_f = \frac{p_{rms} d_f}{2b_h \kappa_f}, \quad (3.41)$$

where d_f is the thickness of the thin film and κ_f its thermal conductivity.

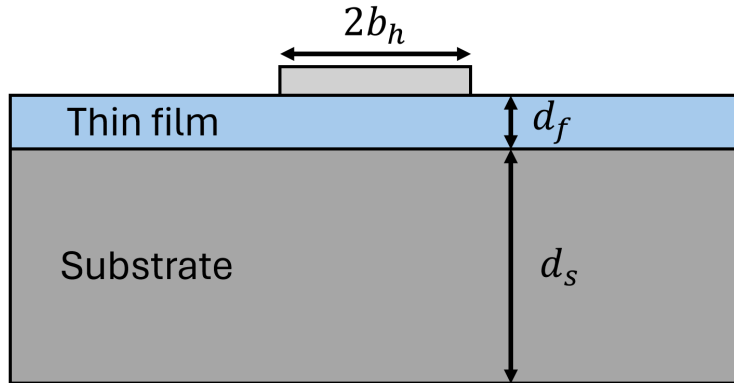
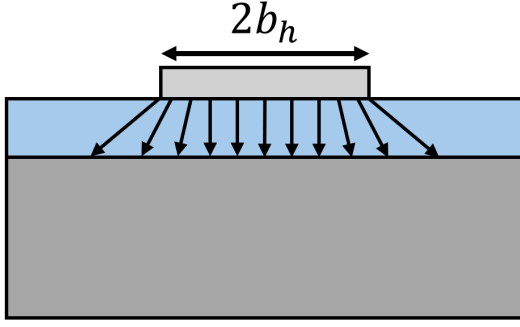


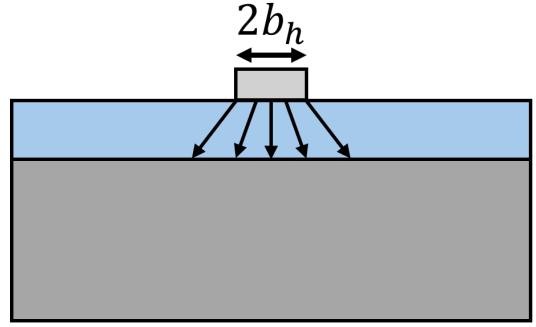
Figure 3.10: Schematic of the thin film case. It consists of a thin film with a thickness of d_f and a thermal conductivity κ_f on top of a thick (possibly semi-infinite) substrate (d_s , κ_s).

[Equation 3.41](#) is valid under the assumption that the temperature profile in the thin film (just under the heater) is one dimensional. This is due to the presence of edge effects because the heater has a finite width.

This can be circumvented by taking a heater wide enough ($b_h/d_f > 5$ for 5% error [\[19\]](#)) or by modifying the effective width of the heater. This second solution comes from the fact that the edge effects widen artificially the heater from the substrate point of view as the heat can spread in the thin film (i.e. 2D heat flow instead of 1D).



(a) Wide heater, mostly 1D heat flow.



(b) Narrow heater, almost only 2D heat flow.

Figure 3.11: Schematic of the effects of narrow heater. A narrow heater has more edge effects compared to its amount of 1D heat flow, effectively widening it from the point of view of the substrate. Black arrows represent (schematically) the heat flow.

Multi-layered system

Determining an approximation for the effective width of the heater and taking into account more complex geometries, such as thick films or more than two layers, requires a new approach to the problem as the one presented until here.

A better heat-conduction model was developed by Borca-Tarsiuc which presents a solution based on a two dimensional spreading of heat in multi-layered system. This is once again under the assumption of uniform heat generation in the heater.

The temperature oscillations, both in-phase and out-of-phase components, at the heater are given by:

$$|\Delta T_{AC}| = -\frac{p_{rms}}{\pi \kappa_{\perp,1}} \int_0^\infty \frac{1}{\mathcal{A}_1(\eta) \mathcal{B}_1(\eta)} \frac{\sin^2(b_h \eta)}{(b_h \eta)^2} d\eta, \quad (3.42)$$

where

$$\mathcal{A}_{k-1} = \frac{\mathcal{A}_k \frac{\kappa_{\perp,k} \mathcal{B}_k}{\kappa_{\perp,k-1} \mathcal{B}_{k-1}} - \tanh(\mathcal{B}_{k-1} d_{k-1})}{1 - \mathcal{A}_k \frac{\kappa_{\perp,k} \mathcal{B}_k}{\kappa_{\perp,k-1} \mathcal{B}_{k-1}} \tanh(\mathcal{B}_{k-1} d_{k-1})} \quad (3.43)$$

$$\mathcal{B}_k = \sqrt{\frac{\kappa_{//,k}}{\kappa_{\perp,k}} \eta^2 + j \frac{2\omega}{\alpha_{\perp,k}}} \quad (3.44)$$

$$\mathcal{A}_n = -\tanh(\mathcal{B}_n d_n)^s. \quad (3.45)$$

In the previous expression, k is the layer number going from 2 (second layer from the heater) to n (substrate). The diffusivity is now considered as anisotropic as the thermal conductivity, such that $\alpha_{\perp,k} = \kappa_{\perp,k} / \rho_k c_{p,k}$.

The complexity of the integral in Equation 3.42 is way higher than the one Equation 3.29 for the mono-layer case which reinforce the principle of using the simpler model possible. This former formula for the temperature oscillations is in perfect accord with the later in the simple mono-layered system.

Equation 3.45 defines the boundary condition on the bottom face of the substrate (last layer). Different values of s refer to different heat sink: $s = 1$ corresponds to an adiabatic condition, $s = 0$ for semi-infinite substrate and $s = -1$ for an isothermal boundary. Both $s = \pm 1$ correspond to finite substrate. Cahill's formula appears in the case $s = 0$.

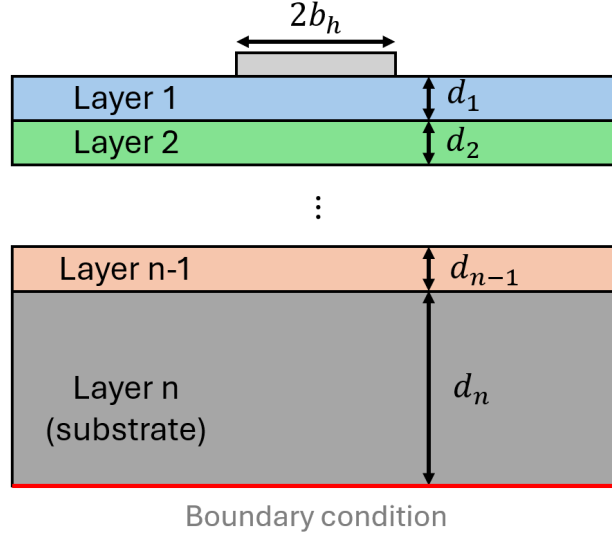


Figure 3.12: Schematic of a general multi-layered system as considered in the Borca-Tarsiuc model. Layer numbers with their width have been annotated to help understanding the numbering.

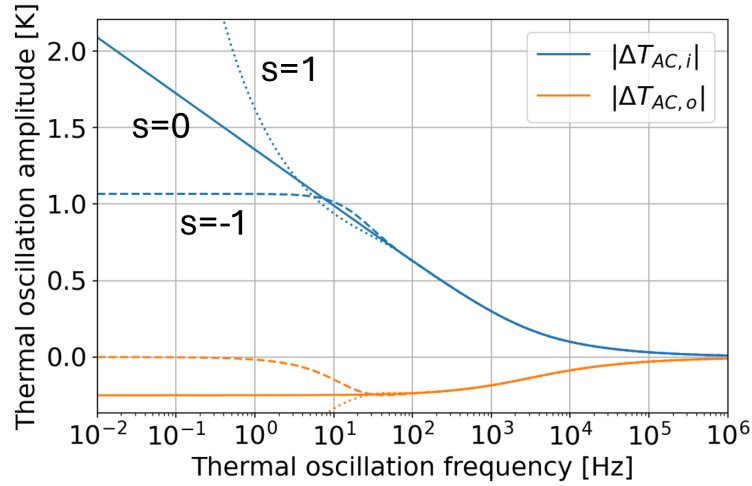


Figure 3.13: Borca-Tarsiuc formula integrated via Simpson integration. The parameters are the same as in Figure 3.6 with a substrate layer thickness of $10\mu m$. The different boundary conditions are represented as solid (semi-infinite), dashed (isothermal) and dotted (adiabatic) lines.

As shown in Figure 3.13, the only differences that appear with the introduction of a finite substrate thickness are in the linear regime. This is due to the fact that for higher thermal oscillation frequencies, the thermal penetration depth is sufficiently low to not reach the bottom surface of the specimen.

In the case of isothermal boundary condition, the thermal oscillations saturate in amplitude and the phase lag disappears. This is caused by the thermal wavelength being substantially larger than the substrate layer thickness cause it to act as a simple 1D thermal resistance. In the case of the adiabatic boundary condition, a similar effect happens. But this time the heat has nowhere to dissipate to, so it comes back to the heater. Going to higher thermal wavelengths just gives more surface for the heat to reflect on, so the amplitude of the temperature oscillations increases.

In reality, this increase is limited by the finite dimensions of the system and external losses such as radiation.

Differential 3-omega method

Quantifying the exact parameters in Cahill's formula (Equation 3.29), for example the thermal diffusivity, while trying to extract the thermal conductivity of a thin film can be hard as we can no longer use the derivative to simplify things (Equation 3.35). This is due to the fact that the term of interest is added to the *original* signal, meaning substrate only, as stated by Equation 3.41.

To circumvent this problem, one can measure different films with varying layer thicknesses. Using those different results, it becomes easy to isolate this additive term by doing a linear regression of the thermal oscillations in the linear regime [20]:

$$\kappa_f = \frac{d_f}{2} \left[\left(\frac{b_h |\Delta T_{AC}|}{p_{rms}} \right)_{s+f} - \left(\frac{b_h |\Delta T_{AC}|}{p_{rms}} \right)_s \right]^{-1}, \quad (3.46)$$

where the subscript s indicates the sample without the thin film and $s + f$ with both.

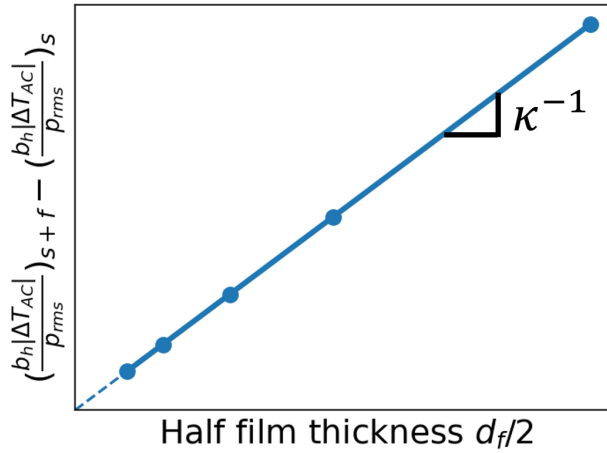


Figure 3.14: Schematic of linear regression of the difference of 3ω measurements as a function of film thickness d_f . The dotted line shows the extrapolation to low film thicknesses.

As shown in Figure 3.14, the difference of measurements on thin film of different thicknesses with one on the substrate only should be linear with the film thickness. However, this linear relationship is under the assumption of constant thermal conductivity (with respect to the film thickness) and neglecting the thermal boundary resistance of the interface thin film/substrate. The latter can induce a shift in the y-intercept of the linear regression. The former will require additional samples of slightly different film thicknesses to better measure the thermal conductivity. By going to small difference of thickness one can hope to measure two samples with the same thermal conductivity while still having a line to regress to.

3.2 Experimental considerations

In this section more considerations on the 3-omega technique will be discussed, this time focused on the setup and practical limits to the formula's presented in the previous section. As the samples were either already available due to previous experiments unrelated to this master thesis or were externally prepared.

3.2.1 Approximations limits

This subsection is based on the chapter 2 of [19].

All considered approximations (e.g. Cahill's formula for thin film, Equation 3.41) have, as their name implies, a domain on which their error is limited. It is important to know such bounds when designing experiment to be able to measure meaningful data which can be analysed at a later date. This is especially true during an experiment as tendencies in the raw data can help spot and resolve possible problems with the setup.

To this end, we need to properly define limits which guarantee a limited error. Two useful threshold to consider are the 1% and 5% error threshold. The later is needed for dealing with trade-off between different limits and relax slow converging issues.

Isothermal substrate

The 3-omega technique when applied to thin films require a good contrast between the thermal conductivity of the substrate and that of the thin film. In particular, the latter should be smaller than the former. This effect is quantified in Equation 3.42 where it is showed that error are on the order of $\kappa_{\perp,f}\kappa_{//,f}/\kappa_s^2$. Usually, thin films are quite thermally resistive due to their small thickness (on the order of microns) as discussed in previous sections. On the flip side, substrate often come in bulk which implies nominal value for thermal conductivity.

When going to thin films of similar thermal conductivity, approximations such as Equation 3.41 may longer work. It is then preferred to fit the theoretical model to the measurement by tweaking its parameter instead.

1D heat flow in thin film

As stated in section 3.1.5, the ideal configuration is a wide enough heater for the edge effects widening the heater to be negligible. In reality however, it is quite rare this is actually the case and those non-idealities should be taken into account.

To that end, it is useful to define the dimensionless heater width: $(b_h/d_s)(\kappa_{\perp,f}/\kappa_{//,f})^{1/2}$.

In the case of isothermal substrate ($\kappa_{\perp,f}\kappa_{//,f}/\kappa_s^2 \ll 1$) for a uniform heat source, Borca-

Tasciuc obtained the following:

$$\Delta T_f = \frac{p_{rms} d_f}{2b_h \kappa_f} S \quad (3.47)$$

$$\beta_f = \sqrt{\frac{\kappa_{//,f}}{\kappa_{\perp,f}}} \frac{d_f}{b_h} \quad (3.48)$$

$$S = \frac{2}{\pi} \int_0^\infty \frac{\sin^2 \lambda}{\lambda^3} \frac{\tanh(\lambda \beta_f)}{\beta_f} d\lambda. \quad (3.49)$$

The quantity S addresses the effect of lateral heat spreading in the film, which can be understood as the ratio $\kappa_{\perp,f}/\kappa_{1D}$ between the effective thermal conductivity and that of the 1D case. For low β_f (<10 , meaning wide heater), the integral in Equation 3.49 approximated to $(1 + 0.38\beta_f)^{-1}$ within a 3% error margin. This leads to a correction in the heater width of the form:

$$b_{eff} = b_h + 0.38 \cdot d_f \sqrt{\frac{\kappa_{//,f}}{\kappa_{\perp,f}}}. \quad (3.50)$$

On the other hand, if the heater is considered narrow, the integral in Equation 3.49 take the asymptotic approximation [19]:

$$S \rightarrow \beta_f \left[0.66745 + \frac{2}{\pi} \ln(\beta_f) \right]. \quad (3.51)$$

Quasi-static heat flow in thin film

As stated in subsection 3.1.2, we assume steady-state for the temperature in the specimen. This makes the assumption that the heat had time to propagate to all the impactful areas of the system. In other words, the heat capacity (in particular of the film) is neglected.

It is necessary consider large wavelength ($\lambda \gg d_f$) to avoid this issue.

Semi-infinite substrate

As stated before, one of the key points of the 3-omega method is that the thermal wave amplitude decays relatively fast. In that sense, having "short" wavelength such that $d_s/\lambda > 5$ keeps the error 1%.

However when this condition is no longer respected, solutions have been presented to account for various substrate boundary conditions in Equation 3.42.

1D heater from substrate point of view

The starting point of subsection 3.1.2 is that the heater can be approximated, albeit finite width corrections, as a one dimensional heat source from the substrate point of view.

To keep error below the 1% threshold, especially when dealing with thin films which can widen the effective width of the heater, it is useful to have $\lambda/b_h > 5$.

Heater infinitely long

Similar to the case of the width, edge effects can appear in the direction of the length as the heater is finitely long.

In the same fashion as most size-related problems, having $l/\lambda > 5$ result in a negligible error of less than 1% [21].

In particular, one should take into account the electrical measurement setup as it is common

to measure the voltage oscillations only at the central half of the heater via the four probes technique. There, a ratio of only 4.7 is necessary.

However, when measuring at full length of the heater, a ratio of 15 is required to keep the error below 1%.

Mass-less heater

The effects of the heater's heat capacity have been quantified to have errors in the order of $(C_H/C)(d_H d_f/\lambda^2)$ [22], where C is the volumetric heat capacity.

It is often the case that the thickness of the thin film is larger or (at most) comparable with the thickness of the heater. This results in the factor $d_H d_f/\lambda^2$ from previous considerations. This leads to relatively small error coming from this non-ideality.

Uniform heat source

As approximated throughout this work and in most 3-omega related analyses, the heater is considered to be an uniform source of heat. This natural assumption might however not be true in practice due to the fact that almost no effort is put in verifying that the Joule heating in the heater is uniform.

The quantification of the error in the case of isothermal substrate has been made in [22]. Under the assumption of wide heater, which should be respected for 1D heat flow in the thin film, the error is less than 3% as long as $\beta_f^{-1} > 4.8$. A similar criterion for the case of narrow heater is $\beta_f^{-1} < 0.06$.

In the case of intermediate regime, meaning $\beta_f^{-1} \in [0.06; 4.8]$, the criterion becomes $(d_H d_f/b_h^2)(\kappa_H/\kappa_f) \ll 1$. This first term should respect the criterion for the same reason of the mass-less heater condition.

Negligible convection and radiation losses

The dimensions of the heater, in particular in the in-plane dimensions, play a huge role on the amount of convection and radiation losses as they depend on the heater surface available for heat transfer with the environment (i.e. everything but the specimen).

Heat is transferred from this surface to its surrounding by a combined heat transfer coefficient h , sum of both contributions: $h = h_{conv} + h_{rad}$.

The radiation part is easily obtained with the Stefan-Boltzmann law:

$$h_{rad} = 4\epsilon\sigma T_{avg}^3, \quad (3.52)$$

where T_{avg} is the average temperature of the sample, ϵ is emissivity of the surface of the sample and σ is the Stefan-Boltzmann constant.

In the case where the thermal resistance of the film dominates of the substrate, the conduction heat flux is $Q_{cond} = 2\kappa_f b_h l \Delta T_H / d_f$ while the total losses (radiation + convection) are, by definition, $Q_{conv+rad} = 2h b_h l \Delta T_H$. This leads their ratio to be equal to the film Biot number: $Q_{conv+rad}/Q_{cond} \approx h d_f / \kappa_f$. Using typical values for this last expression ($d_f \sim 1\mu m$ and $\kappa_f \sim 10W/m.k$) shows that the losses are below the 1% threshold for a heat transfer coefficient of less than $1kW/m^2.K$, which is very easily satisfied.

In the case where the thermal resistance of the substrate dominates, we go back to the fact that the heat spread is limited by its wave-length λ as the amplitude of the thermal oscillations decays rapidly. By similar looking relations as in the previous case for the different heat flux, this time involving the thermal penetration length, we get a ratio $\frac{Q_{conv+rad}}{Q_{cond}} \approx \frac{h\lambda}{2\kappa_s}$. Using typical values of $\lambda \approx 100\mu m$ and $\kappa_f \approx 150 \text{ W/m.K}$, the losses are below the 1% threshold for a heat transfer coefficient of less than $30\text{kW/m}^2\text{.K}$, which is very easily satisfied.

3.2.2 Measurement setup

In order to generate and measure a 3-omega signal, a **Zurich Instrument MFLI Lock-in amplifier** is used. There are three configurations:

- One without any external circuit.
- One with a Wheatstone bridge (full).
- One with a Wheatstone bridge (half).

They are ordered by the quantity of external circuit and lab equipment required in parallel with the lock-in from first (the least) to last (the most). Each of them has its pro's and con's. The first two configurations were used for the measurements.

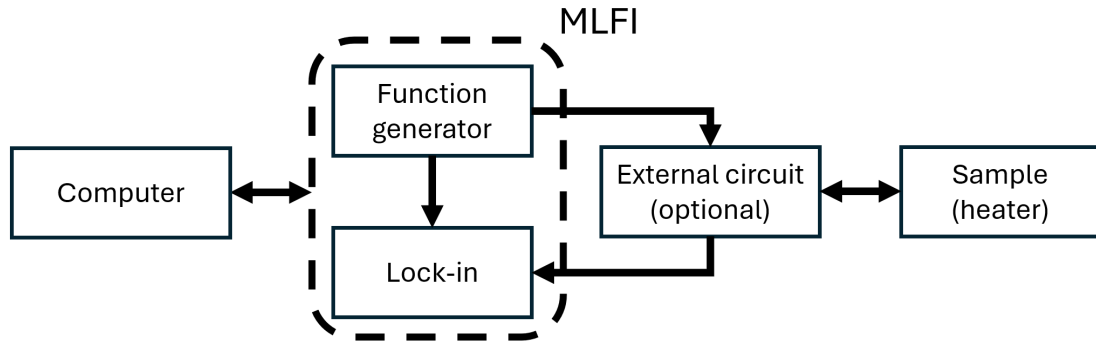


Figure 3.15: Schematic of the setup used for measurement. The MLFI is used as both signal generator and lock-in for measuring the third harmonic component. This signal is generated in the sample with the help of an (optional) external circuit. The MLFI is controlled by a computer which also retrieves data for further analysis.

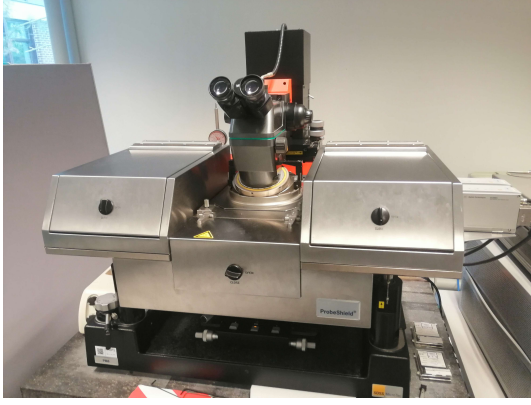
The sample is a thin rectangular heater of either aluminum or nickel deposited on top of a multi-layered wafer. The details of the shape of this heater and the different kind of wafers will be explained in [subsection 3.3.1](#).

The wafer is held via vacuum suction to a thermal chuck (to control the temperature) in a **PM8PS Low Signal probe station**, which offers four manually controllable probes.

3.2.3 Lock-in amplifier

One of the key challenges of the 3-omega technique is to efficiently isolate the 3-omega component of the measured electrical signal from its first harmonic. This must be done in an automatic fashion as the measurement needs to be done over a wide range of frequencies, spanning over multiple orders of magnitude.

This makes it impossible to use a simple high-pass filter (HPF) as its order and cut-off



(a) PM8PS low signal probe station.



(b) Zurich Instrument MFLI Lock-in amplifier.

Figure 3.16: Instruments used for the 3-omega measurements.

frequency need to be adjusted continuously while sweeping in frequency. Indeed, if we manage to setup the HPF for a certain frequency, tripling it (during the sweep in frequency) will render it useless as the first harmonic will now be in its pass-band.

To alleviate this problem, one can use a device called "Lock-in amplifier". Its goal is to extract from a signal a narrow range frequencies (ideally only one) which is defined by a reference signal. Also, it should be able to discriminate signals relatively close in frequency.

Mixing signals

The working principle of this device is as follows:

If we multiply two sines together, we get the addition of two sines back. One of them has a frequency equal to the difference of the two input signals while the other has one which is equal to the addition instead.

$$\cos(\omega_a t) \cdot \cos(\omega_b t) = \frac{\cos((\omega_a - \omega_b)t) + \cos((\omega_a + \omega_b)t)}{2}. \quad (3.53)$$

More importantly, if they have the same base frequency, the resulting signal has a DC component and sine oscillating at twice the input frequency.

The key point is that every electrical signal can be decomposed as a sum of sines and cosines, which is called its Fourier series:

$$V(t) = V_{DC} + \sum_{k=1}^{\infty} A_k \cos(k\omega_s t) + B_k \sin(k\omega_s t), \quad (3.54)$$

where ω_s is the fundamental frequency of the signal and A_k and B_k are complex coefficients. In our case, we can re-write this sum to only two components, discarding higher order terms, which correspond to non-idealities and noise:

$$V(t) = V_{1\omega} \cos(\omega t) + V_{3\omega} \cos(3\omega t). \quad (3.55)$$

Multiplying [Equation 3.55](#) by a third harmonic reference signal and applying [Equation 3.53](#)

we get:

$$2V(t) \cos(3\omega_s t) = V_{3\omega} \left[1 + \cos(6\omega_s t) \right] + V_{1\omega} \left[\cos(2\omega_s t) + \cos(4\omega_s t) \right]. \quad (3.56)$$

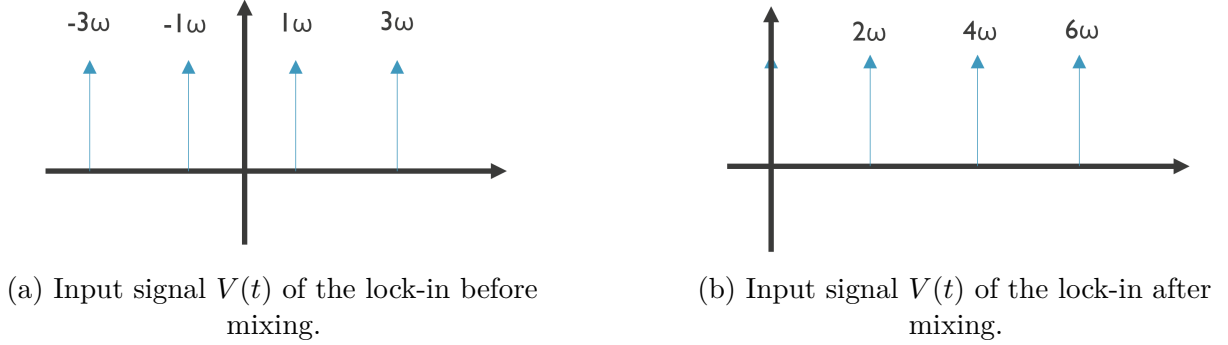


Figure 3.17: Schematic of the frequency of the input signal of the lock-in before and after mixing with a third-harmonic signal

Low-pass filter

As seen in [Equation 3.56](#), we get a DC component, which contains the part of the signal we're interested in, with harmonics of twice the fundamental frequency of the input signal. We can use a low-pass filter (LPF) to retrieve the signal of interest. The good part is that this time we only need to adjust the cutoff frequency of the filter without worrying about it being centered, which greatly simplifies the task.

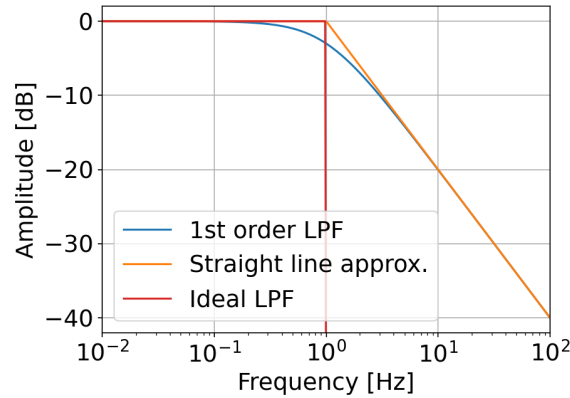


Figure 3.18: Example of a first order low-pass filter with a cut-off frequency $f_c = 1\text{Hz}$. Its roll-off factor is of -20dB/dec meaning the signal is attenuated by 20dB every decade (i.e. every time we multiply the frequency by 10 after the cut-off).

There are two important parameters to a LPF: the cut-off frequency and its order. The cut-off frequency is the frequency at which the amplitude of the attenuation is of $1/2$, or about -3dB . It sets where the attenuation starts to take effect.

The order gives the amount of additional attenuation the LPF applies every decade (or octave). For a first order filter it is -20dB/dec . For higher order filters, this attenuation increases. For example, in the lock-in used in this master thesis, the highest order of filter is

8, resulting in an attenuation of -80dB/dec.

By approximating that the first harmonic component of the signal is 1000 times stronger than the third harmonic we're interested in. This factor is equivalent to +30dB. A good rule of thumb for a signal to reject another is that they should have 60dB of amplitude difference. With an eighth order filter, this can be achieved for difference between the first and third harmonic if the cut-off frequency is set at approximately one decade before the fundamental frequency of the signals (after the signal mixing).

Locking in on a signal

Now that we have the signal of interest, we need to integrate it to get its amplitude. A signal is said to be periodic if it repeats after a precise amount of time: $f(t) = f(t + \tau_s)$ where τ_s is its period in seconds. Taking the particular case of sines, this period directly translate into the the frequency of oscillation $f_s = 1/\tau_s$, which is also called the fundamental frequency. In other words, the lower the frequency, the longer the period of the signal. This means that if we want to integrate a signal over several periods to accurately measure its amplitude and phase, we have to wait longer for low frequencies.

Also, due to the small nature of the third harmonic signal, averaging is required. This means taking a possibly high number (1000 to 10k) of samples, i.e. the integration procedure discussed just before, and average their result to decrease the uncertainty tied to the noisy nature of the measurement.

Due to these two facts, a single sweep over three orders of frequency can take time in the range of minutes to low tens of minutes for accurate results.

3.2.4 Wheatstone bridge

One of the key problems with the 3-omega technique is that even though the third harmonic electrical signal picked has a different frequency than the first harmonic signal (due to the DC temperature rise as in [Equation 3.5](#)), the former has an amplitude which is orders of magnitude lower than the latter. This problem which might seem trivial at first glance is in fact of major concern.

This is due to the way that the lock-in works: the signal processing is done via a set of complex component, such as mixers. Those types of component have defined ranges for input and output. In other words, signals that need to be processed are limited in amplitude. This range of input amplitude will define the noise floor, i.e. the minimum amplitude a signal needs to have to be picked up by the instrument.

So, we need to have those two amplitudes as close as possible (the maximum one needs to be greater than of the signal to avoid saturation) to have the best precision on the data signal. However, as shown in [Figure 3.19](#), the output of the final low pass filter (in green) is after the range selector (in red). This means that the range of the data signal is dictated by the amplitude of its highest harmonic.

As stated before, the first harmonic (which is useless for determining the properties of the specimen) is orders of magnitude greater than the third harmonic. This means that the range is not suited to measure the latter harmonic leading to poor precision.

Even with a good precision lock-in, it is necessary to use an external circuit to cancel the

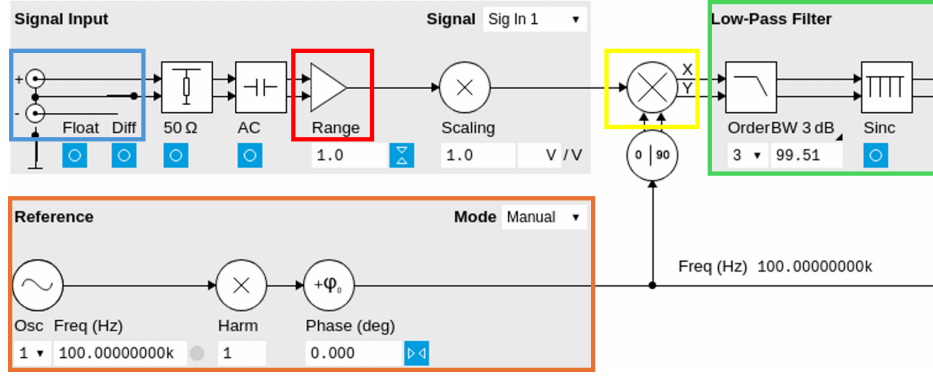


Figure 3.19: Screenshot of the lock-in process in the GUI of the MFLI Lock-In. In blue is the input signal (differential or not), in red the range selector, in yellow the signal mixer, in orange the reference signal generator and in green the final low pass filter, which is the output.

$V_{1\omega}$ component of the signal before processing. The one used in this work can go to up to μV of precision for the lowest range of 10mV.

To this end, an external circuit called "Wheatstone bridge" is used.

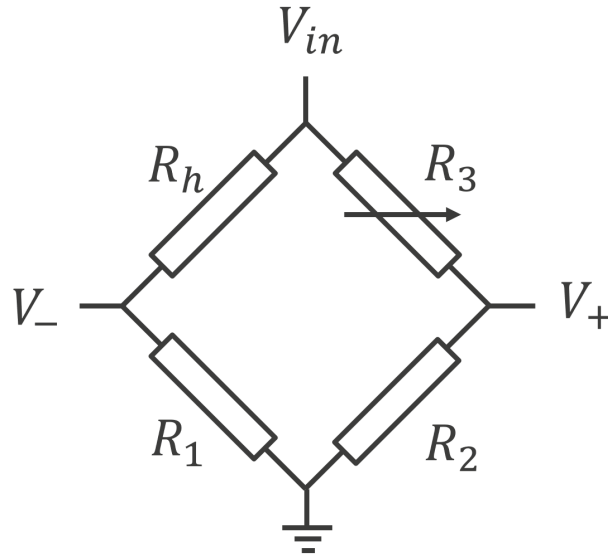


Figure 3.20: Schematic of a Wheatstone bridge. Resistors R_1 and R_2 are known, R_h is the unknown resistor and R_3 is a variable resistor. Balancing is made by reaching $V_+ = V_-$ by tuning R_h . V_{in} is an arbitrary biasing signal.

As shown in [Figure 3.20](#), the Wheatstone bridge is composed of four resistors: two of known value (R_1 and R_2), the unknown resistor (R_h) and a variable resistor (R_3). It works by tuning R_3 in such a way that the difference $V_+ - V_-$ reaches zero. The signal V_{in} is a simple biasing signal used to make V_+ and V_- different than zero.

We can write the different voltages using Ohm's law:

$$\begin{aligned} V_+ &= V_{in} \frac{R_2}{R_2 + R_3} \\ V_- &= V_{in} \frac{R_1}{R_1 + R_h}, \end{aligned} \quad (3.57)$$

such that

$$V_+ - V_- = 0 \Leftrightarrow R_3 = R_h \frac{R_2}{R_1} \quad (3.58)$$

The use of this circuit is around the fact that we can enforce the generation of third harmonic component in the heater, here R_h . If we chose a set of known resistors (R_1 , R_2 and R_3) to have very low TCR (or equivalently very stable from a thermal point of view), there will be perturbation generated only in the left branch of circuit, breaking the balance previously achieved.

If we supply the circuit with a voltage oscillation at a fundamental frequency $f_s = \frac{\omega_s}{2\pi}$, we can balance the bridge around the room temperature values of the resistors:

$$R_{3,0} = R_{h,0} \frac{R_{2,0}}{R_{1,0}}. \quad (3.59)$$

By the definition of TCR, each of the four resistor will experience a change in the value of their electrical resistance due to the oscillating current going through them.

By performing some algebra and using the fact that the TCR of all of the known resistors is way lower than the one of the heater, we arrive at the following relationship between the difference of voltage in the middle the bridge $\Delta V = V_+ - V_-$ and the third harmonic component that we're interested in:

$$\Delta V = V_{3\omega} \frac{R_{1,0}}{R_{h,0} + R_{1,0}}. \quad (3.60)$$

One other important quantity to compute is the amount of current delivered to the heater. If we input a current I_{in} through the bridge, going from the V_{in} port to the ground port, we have in the left branch:

$$I_h = I_{in} \frac{R_{2,0}}{R_{1,0} + R_{2,0}}. \quad (3.61)$$

By analysing [Equation 3.61](#), we can see that the greater the ratio $R_{2,0}/R_{1,0}$, the more current goes into the branch with the heater. Conversely, from [Equation 3.58](#), the higher this ratio is the greater the variable resistance R_3 needs to be.

In practice, variable resistors and the heater have the same range of resistance, but sometimes the latter is more resistive than the latter. This means that more than half the input current will go to the right branch, which is wasted current. And even more problematic than that, higher current means higher variation of temperature and as such, higher variation in the resistance due to the TCR in the right branch. This can lead to the unbalancing of the bridge through time as the resistors heat up, which is to be avoided.

3.2.5 Half bridge

To this end, another configuration of the Wheatstone bridge can be used [\[23\]](#).

This configuration as shown in Figure 3.21 works by using only one known resistor of low TCR and thus creating a reference signal containing only the first harmonic of the signal. This resistor is variable to accommodate process variations in the electrical resistance of the heater or simply different heaters.

Some works [24] even go to the point of tuning in this variable resistor automatically via computer-driven feedback loops. Such setups are however much more complex and may introduce error.

This configuration allows the introduction of another module to boost the signal amplitude before feeding it to the lock-in amplifier to boost the signal to noise ratio.

Compared to the full bridge configuration, this one requires the use of active components which can introduce noise or distortions and require some kind of power supply. It however suffers less from TCR-related problems (only one resistor needed) and gets rid of the waste of current as there's only one branch through which it can propagate.

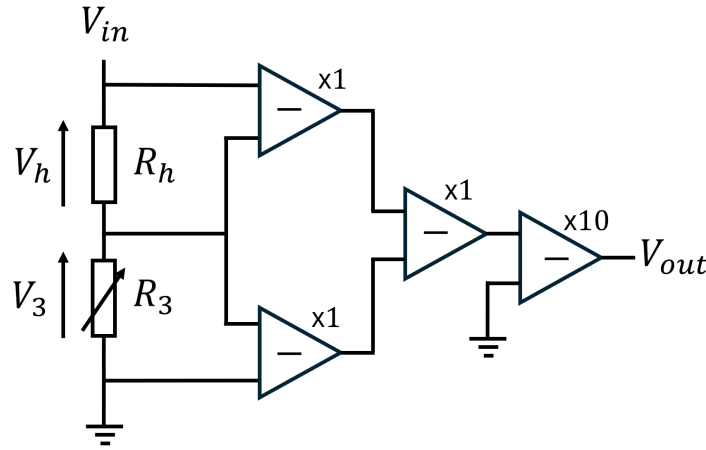


Figure 3.21: Wheatstone bridge in half bridge configuration. The triangles represent low-noise subtraction module with an amplification of either one (x1) or ten (x10).

Note that the last two modules can be taken out so that the two outputs of the first two are directly fed to the differential input of the lock-in. This reduces the amount of noise generated in the external circuit at the cost of the third harmonic voltage not being amplified before being fed to the lock-in.

3.2.6 Four point probing

One of the main problems of the way the heater is hooked up to the rest of the system is that there is parasitic resistances between the measurement points. Ideally, (jumper and coax) cables between component are perfect in the sense that they have 0 inductance and 0 electrical resistance.

However, in the real world those cables are slightly imperfect. The most noticeable non-ideality is the non-zero electrical resistance which can reach in the worst cases up to ohms. Considering the fact that the heater resistance is in the range of tens of ohms, the impact of those (unavoidable) imperfections can be non-negligible.

As we're only interested in voltage drop across the heater, we can use a well-known technique called "four probes measurement" instead of the simpler two-probes measurement.

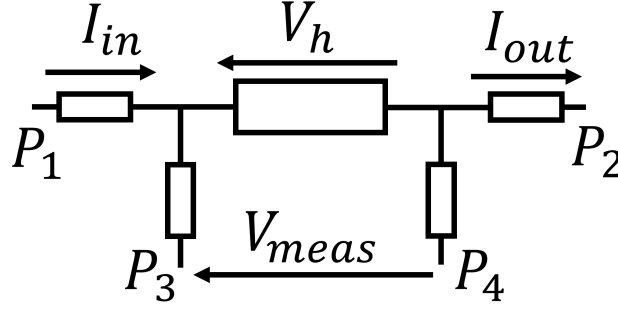


Figure 3.22: Schematic of four probes measurement. The unlabelled resistors are parasitics due to the non-ideal cables. As $I_{in} = I_{out}$, the measured voltage V_{meas} between probes P_3 and P_4 is the same as the true voltage V_h of the device under test.

As shown in Figure 3.22, cables introduce parasitic resistors in between the specimen (big resistor in the middle) and the probes (labelled P_1 through P_4). When doing voltage measurement, we can assume zero current going into the measuring probes (P_3 and P_4). This means that the going in the system I_{in} through probe P_1 is the same as the one going out I_{out} via probe P_2 . This means that the measured voltage V_{meas} is the same as the voltage that we want to measure V_h .

So the way the heater R_h is hooked up to the Wheatstone bridge as shown in Figure 3.21 is done via four probes. This is also the way the specimen is measured when using no external circuit.

However in the configuration of the full bridge as shown in Figure 3.20, this method can't be applied as don't measure the voltage across R_h . This is however not an issue of major concern due to the nature of cables: they have high thermal conductivity [25] and not so high TCR (comparable to aluminium) [26]. This means that those cables stray from room temperature only slightly.

3.3 Results

In this section the application of all the previous part of this chapter will be discussed. The main goal of the developed setup was to measure the thermal conductivity of thin film (possibly multiple layers) on silicon but as we'll see, the results will be only limited to try and measure the (known) thermal conductivity of the substrate only.

3.3.1 Available samples

The provided samples were samples coming from UCLouvain (quartz sample only) or from IMEC (thin film on silicon substrate).

CPW lines

All of the IMEC samples were initially patterned with different structures for RF testing, namely co-planar wave-guide (CPW) lines. These structure where made of relatively thin aluminium, which can be exploited for 3-omega measurement.

As shown in Figure 3.23, those CPW line structures are composed of three conductive traces (gray areas): the central one is where the signal propagates while the other two are ground.

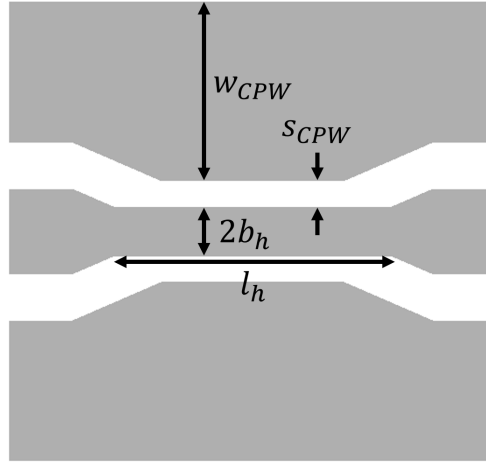


Figure 3.23: Schematic of a CPW line used for testing with the different dimensions highlighted. The top and bottom gray areas are the ground while the central gray area is where the signal propagates.

b_h and l_h usual width and length of the heater respectively, the h subscript in the length used here only to differentiate it from the total length of the structure. But in practice those two lengths can be approximated to be the same as the pads are much smaller (a few tens of microns in side-length) compared to the size of the structure (a few millimeters in length). The quantities w_{CPW} and s_{CPW} are the width of the ground line and the spacing between the ground and signal lines respectively. The structure is symmetric (folding symmetry) along its two major axes.

In the case of 3-omega, the CPW lines are not ideal because the signal integrity is not lost (the frequency is fortunately too low for that) and we can *only* do two point measurements with them. This second point can be somewhat alleviated by placing two probes on each side of the signal trace but it is no easy task to do, especially with a fully manual probing station, as shown in [Figure 3.24](#).

Two-dimensional FEM simulations (approximating the length of the heater as infinite) showed that the impact of side ground does not impact significantly the behaviour of the 3-omega response of the sample for all ranges of frequencies (i.e. from 10Hz to 1MHz).

Re-patterning structures

Due to the difficulty of probing those small pads, the decision to re-pattern the structures was quickly reached. This could allow the use of custom structures, namely four probe structures with custom sizes and the use of other metals.

Aluminium is a good material with acceptable levels of resistivity, i.e. around ten ohms for typical structure sizes ($10\mu m \times 2mm \times 200nm$ respectively for the width, length and thickness). Also, it has a relatively good TCR value of around 0.004 K^{-1} at room temperature. However, nickel while being about two to three times more resistive (which is tolerable) has a better TCR value of around 0.006 K^{-1} at room temperature.

The re-patterning was thus done on all the samples by [Incize](#). All of the samples were re-patterned using nickel except with the Quartz sample for which aluminium was used. This different choice for this single sample is a consequence of the fact that the decision to

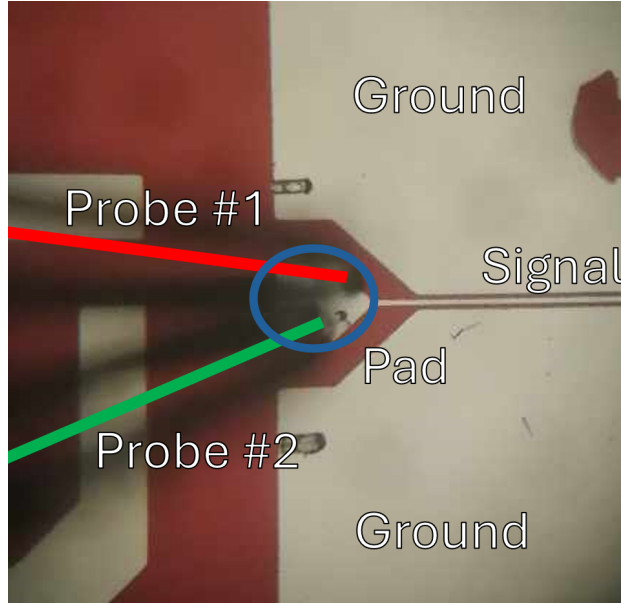


Figure 3.24: Photograph of two probe connected on the same pad of a CPW line. The green and red lines indicates the double wired probes while the blue circle highlight the small pad. The small black line on the top and bottom of the pad are scratches of previous RF measurement (not done by me).

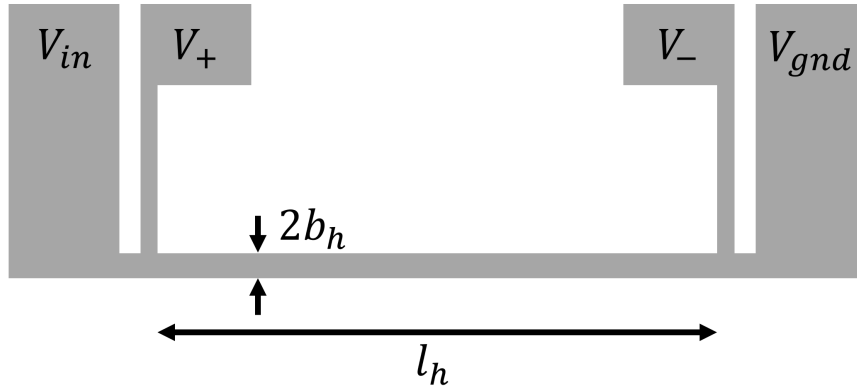


Figure 3.25: Schematic of a four probe structure patterned on the surface of the sample. Typical values for the length l_h and width $2b_h$ are 2mm and $10\mu m$ respectively. The V_{in}/V_{gnd} pair of pads is for the input signal and the V_+/V_- pair is for measuring the drop in voltage across the heater.

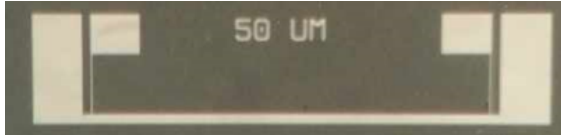
switch to nickel was made after its processing.

Fortunately, only one of the samples suffered from serious patterning issues, as shown in [Figure 3.26b](#).

List of samples with details

Two of the wafers were not usable do to processing problems. One was subject to delamination (Si only wafer) and another one, as mentioned before, subject to bad patterning. Only the working ones are referenced below.

All the of the sample have a substrate layer thickness of around 1mm, including the quartz sample.



(a) Good patterning.



(b) Bad patterning.

Figure 3.26: Examples of good and bad patterning of four-probes structure on two different samples. Notice that on the bad patterning example there is no trace between the heater and the V_+/V_- probing pads.

The stack structure of the Si substrate samples is the same as shown in [Figure 2.1](#).

- Sample A: Quartz substrate with aluminium structures.
- Sample B: Si substrate with 5s of AlN NL growth with nickel structures.
- Sample C: Si substrate with 15s of AlN NL growth with nickel structures.
- Sample D: Si substrate with 300nm GaN channel with nickel structures.
- Sample E: Si substrate with 100nm GaN channel with nickel structures.

The AlN NL (nucleation layer) treatment time in seconds refers to the amount of time a precursor is used. This directly affects the property of the AlN [7]. It however doesn't change its layer thickness.

Structure sizes

As stated in [subsection 3.2.1](#), the length of the heater needs to be at least in the order of a millimeter. Thus, the heaters are either 1, 2 or 4mm long. The different values ensure a possibility to change the value of the total resistance of the heater without changing the width, which has a direct impact on the measurements.

The width ranges from $1\mu m$ to $50\mu m$ in a logarithmic like fashion, meaning there's more structures with small width. This is to account for different layer properties which may require narrow or large heaters.

The thickness has been chosen to be smallest possible, i.e. 200nm, as the resistivity of aluminium (and also nickel) is a bit too low.

Using a resistivity of $2.7 \times 10^{-9}\Omega.m$ for aluminium with a device size of $200nm \times 10\mu m \times 1mm$ (thickness, width, length) we get a total resistance of 13.5Ω . Higher resistances (hundreds of ohms) could be used but they might require additional care from the power supply side of things (higher voltages required for the same power delivered to the heater) and higher values of variable resistors.

This second point can be resolved with the use of full Wheatstone bridge by using a R_2/R_1 different than one. This change however results in a lower current in the heater branch as discussed before and should be accounted for.

3.3.2 TCR measurement

The TCR value of the structures is one of the most important factors in getting accurate 3-omega results as it is the conversion coefficient between electrical signals and the amplitude of thermal oscillations.

As stated before, it is a first order approximation of the change in resistance with temperature. It can be expressed as the following formula:

$$\beta_h = \frac{1}{R} \frac{\partial R}{\partial T}. \quad (3.62)$$

Approximating this value to be constant over small interval of temperature, for example less than 10K, we can measure the value of a resistor (in our case a heater) at different temperatures and find the best line fit. We can then apply [Equation 3.62](#) to find the average value of TCR of a given sample.

As this process requires heating up the sample at several temperature steps, it is quite time consuming. TCR measurement are quite insensitive to process variations and so it is good

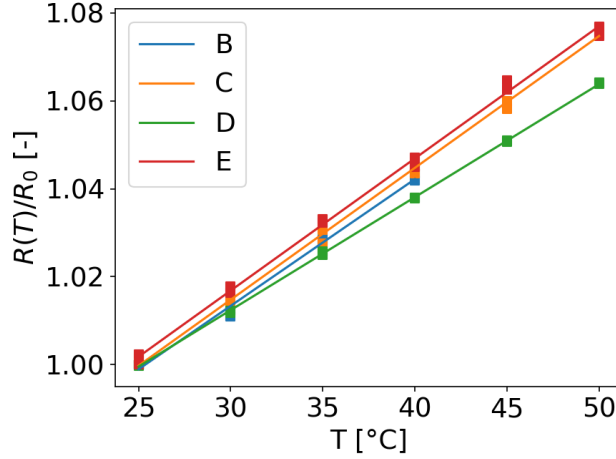


Figure 3.27: Variation in (normalized) resistance over temperature for Si substrate samples with best line fit. R_0 is the value of the resistance at 25°C.

enough to do it only once per sample. It is however best practice to use nearby structures for further 3-omega measurements just to be sure, especially in the case of large wafers.

As shown in Figure 3.27, the TCR for the different samples is pretty close. The slope of the curves vary between 0.0027 and 0.003 K⁻¹, which is lower than the value of 0.006 K⁻¹ found in literature.

The same procedure was applied to the Quartz sample which yielded a value of 0.003 K⁻¹ which is also lower than in the literature (0.004 K⁻¹).

Both values in found in the literature are values for bulk material, which is clearly not the case here as we have ~ 200nm thick metal strips. This difference is known, as discussed before, to have a huge impact on the thermal properties of the material, which is most probably also the case for TCR.

3.3.3 Thermal conductivity measurement

Quartz sample

In the case of the quartz sample, 2mm long heaters were used. This was to remediate the low resistivity of aluminium.

For the width, they were each 5μm wide to achieve a resistance value of at least 10Ω. in this case, the measured resistance was around 16Ω for the three samples. This value is to reach acceptable levels of input power p_{rms} while having a resistance not too low as to not be too much affected by parasitics.

One important note is that as the amplitude of the thermal oscillations is inversely proportional with the substrate thermal conductivity, the measured third harmonic is not that small compared to the first harmonic in the case of low conductivity substrate. As it is the case for quartz, the resulting 3-omega signal is in the range of 50μV to 100μV which can directly be picked-up by the lock-in amplifier.

This means that in this case using a Wheatstone bridge can be avoided. In such cases, it is better to do without as this allows us to use no external circuit which can be source of noise, in part due to the cables between the sample and the circuit itself. Also, this limits the power loss in the passive components of the bridge (i.e. balancing resistors) which furthers

improve the amplitude of the third harmonic compared to the noise which is on the order of $0.1\mu V$ to $1\mu V$. This however comes with the price of a high first harmonic. But again, in this case it can be suppressed by the lock-in.

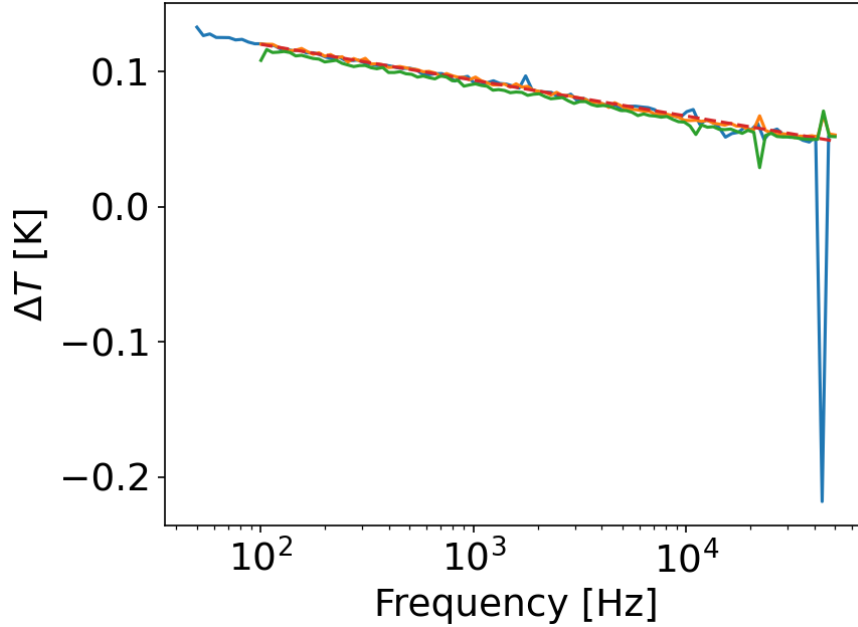


Figure 3.28: Amplitude of the in-phase component of the amplitude of the thermal oscillations in the linear regime for different heater width. The red dotted line shows a linear regression of the data.

As shown in Figure 3.28, the results are pretty consistent with the different samples on the same wafer. While it would have been preferable to have access to another wafer to test device variability, there was unfortunately no other made out of Quartz.

In any case, extracting the thermal conductivity of those measurement using the slope method as in Equation 3.35 yielded the following thermal conductivity: 1.52 ± 0.16 W/m.K. This value is slightly higher than the accepted value of 1.38 ± 0.04 W/m.K.

Silicon samples

In the case of the silicon samples, a Wheatstone bridge is required to pickup any signal as the third harmonic as an amplitude in the range of $10\mu V$ at most. In this work, only the full bridge configuration realised and so is the only one available.

All the nickel structures where found to be much more resistive than what theory predicts. The exact measured values can be found in **annex:R** but in summary, for a $200\text{nm} \times 10\mu\text{m} \times 2\text{mm}$ (thickness, width and length) nickel heater the resistance was found to be $1530 \pm 70\Omega$ while the theoretical value should be of 70Ω (value for bulk nickel). Those results are consistent over various wafers and heater dimension, i.e. same resistivity of around $1.53 \times 10^{-6}\Omega\cdot\text{m}$ instead of the bulk value of $7 \times 10^{-8}\Omega\cdot\text{m}$.

The difference might be explained by a change in the properties of Nickel in the case of thin films, but literature on this specific case wasn't found. This drastic change is pretty strange due to the fact that the aluminium samples were not subject to such dramatic changes.

This resulted in the Wheatstone bridge to have a ratio of R_2/R_1 to be 0.1 instead of 1 for the variable resistor of 500Ω max to be able to balance with the heater.

In any case, tests were performed on all four silicon substrate wafers. For samples B to D, tests were performed on $5\mu m$ and $10\mu m$ wide heaters which all were 2mm long. This change of width should not have an impact on the extraction of the thermal conductivity of the substrate via the slope method but can help with determining the thermal conductivity of the above layers.

Note that the width of $5\mu m$ is, in theory, large enough for the first significant layer to experience quasi 1D heat flow, which should allow for the extraction of its thermal conductivity via the Borca-Tarsiuc model.

However, the power delivered to the heater was found out to be insufficient for the thermal oscillations to be big enough for the setup to function properly. This resulted in the extracted thermal conductivity of silicon to be of almost 0 for the sample B, C and D.

The sample E on the other hand had an even stranger resistivity, higher than the rest but constant throughout the wafer. It should be noted than in its case, the surface finish was a bit strange in the sense that it is not smooth, as shown in [Figure 3.29](#).

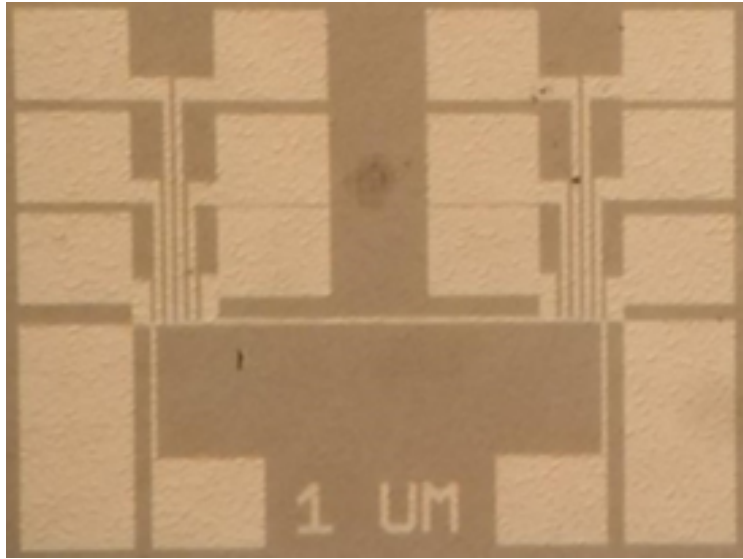


Figure 3.29: Photography of the surface roughness of sample E via an optical microscope. This roughness is best seen on the pads as the contrast is better there.

This fact forced the use of much larger heater width which decreased the resistance, to the point of being smaller than the maximum value of the variable resistor, leading to a use of a factor of $R_2/R_1 = 1$. This means that half of the power is directed to the branch with the heater which resulted in enough power p_{rms} being dissipated in the heater.

As shown in [Table 3.2](#), the calculated values for the thermal conductivity of the substrate (Si) substantially differ from the accepted value of 156W/m.K . Those results were generated by sweeping in frequency between 100Hz and 20KHz.

k [W/m.K]	R [Ω]	I_0 [mA]	p_{rms} [W/m]
96.090	347	0.9899	0.1700
68.052	347	1.980	0.6801
81.310	347	4.950	4.251
20.460	684	0.5657	0.1094
106.223	684	1.131	0.4378
88.223	684	2.828	2.736

Table 3.2: Extracted value of the thermal conductivity of the Si substrate for sample E.

As we're dealing with a multi-layered system, it is reasonable to ask the contribution of those upper layers.

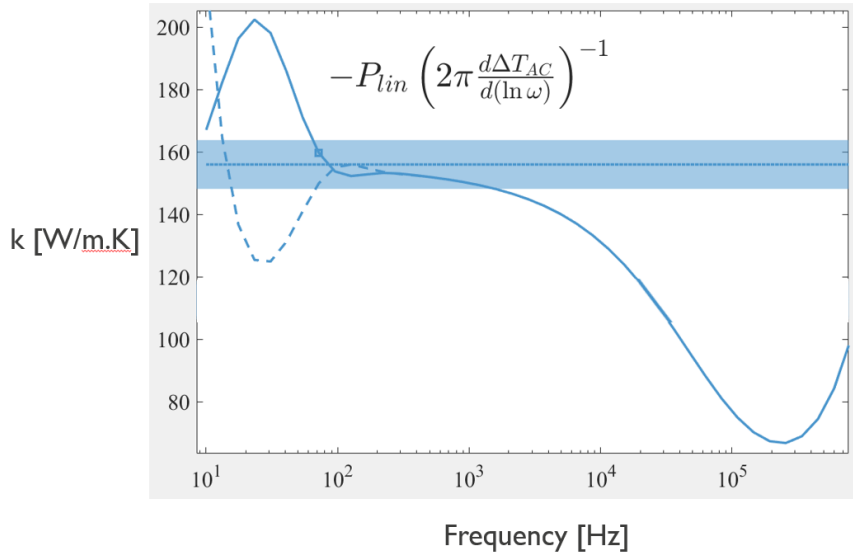


Figure 3.30: Simulation with the Borca-Tarsiuc model of the 3-omega response of the sample E. In this graph is represented the extracted value of thermal conductivity of the substrate via the slope method.

As seen in [Figure 3.30](#), the extracted thermal conductivity of the substrate via the slope method, as done in [Table 3.2](#), should not substantially differ from the accepted value, highlighted as a blue strip in the figure.

The most sensible explanation for this behaviour would be the presence of unaccounted parasitics.

However, even we add a series resistance in series with the power source, the change in the measured thermal conductivity would be of only 10 W/m.K.

This may also come from the power delivered to the heater being, in fact, too low. As the lock-in was reaching its maximum power output, this hypothesis couldn't be tested.

One last piece of limitation encountered was the presence of a inexplicable inductor-like behaviour of the circuit. Even though only resistors, (short) jumper cables and coax cables were used for the external circuit and connections between it, the prober and the lock-in, a rise in first harmonic voltage was noticed when increasing the operating frequency, in a linear fashion, at the output of the Wheatstone bridge.

As shown in [Figure 3.31](#), this behavior is almost perfectly linear and only affects the out-of-phase component of the signal. Extracted values show a equivalent inductance of 0.3mH to

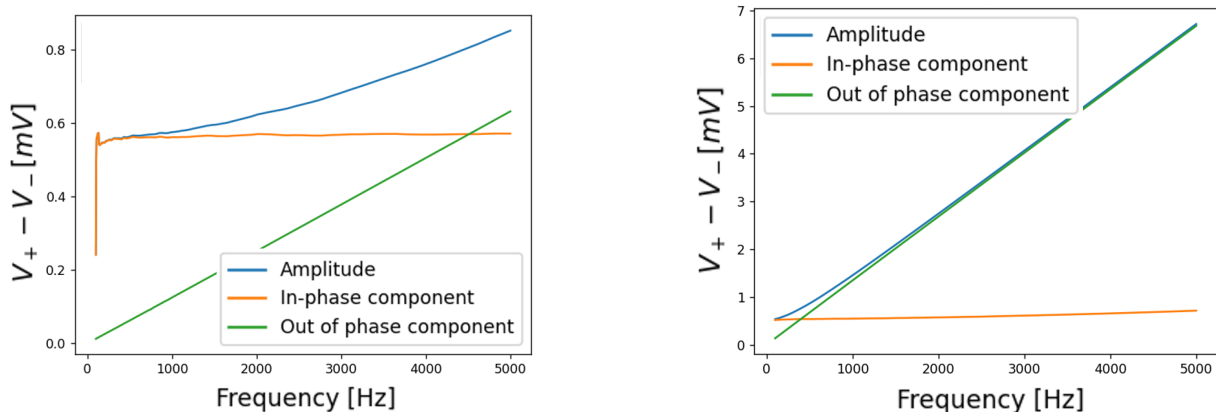


Figure 3.31: Examples of inductor-like behaviour appearing at the output of the full Wheatstone bridge. The blue, orange and green lines represent the total amplitude of the signal, its in-phase component and out-of-phase component respectively.

3mH depending on heater measured.

This behaviour doesn't seem to impact the measurement directly. However, it can lead to a saturation of the lock-in if the amplitude of the signal increases further than the range of the analog to digital converter (ADC).

3.3.4 Discussion

Conclusion

The modelling of temperature and heat distribution is no trivial task. This is the case even when considering simpler configuration such as a one dimensional heater on a semi-infinite sample. However, through mathematical modeling it is possible to arrive as numerical models, such as the finite element methods or recursive integrals for simpler geometries, efficient enough to be run on laptops in a moderate amount of time.

Using to models it is possible to define regimes in frequency in which the behaviour of the thermal waves is linear with the logarithm of the frequency.

Using this information, thermal conductivity can be extracted from electrical measurement using the property of resistors to change their value depending on temperature.

In this master thesis, a setup for this technique called the 3-omega technique has been developed to characterise the thermal conductivity of thin films of material in GaN-on-Si transistors.

However, due to technical difficulties with the technique, simpler measurement were performed.

As this technique is proven to be more difficult to be performed on high thermal conductivity materials such as silicon, the first tests were performed on Quartz.

Those tests were proven to be pretty useful on the debugging of early setups and ultimately lead to the successful measurement of the thermal conductivity for this type of substrate.

However, the setup in its current form wasn't able to measure the higher thermal conductivity of silicon, let alone the thin films deposited on top. More efforts are thus required to be able to accomplish this goal and attempt this initial one.

Future work

In order to improve the workings of the current apparatus, it would be useful to test the half Wheatstone bridge configuration. As discussed in the case of the silicon samples, the current configuration (full bridge) uses too much power in its right branch which leads to a non-negligible drop in effective power delivered to the heater p_{rms} . This has the consequence to directly lower the amplitude of the thermal oscillations. As the third harmonic is already small, making it even smaller makes it comparable to sources of noise, such as thermal noise. This configuration however comes at the price of using an external power supply. It would be wise in that case to design an external circuit on a pcb.

To this goal, this [useful resource](#) available online can be a good baseline as it details every aspect of the project, for example including schematics with details of such a pcb.

I unfortunately found out about it way too late, and as such couldn't implement and test it on available samples.

One other possible way to improve results would be to use the differential 3-omega method as it would be able to better discriminate individual layers from the rest. This however requires the production of multiple wafers with different layer thicknesses which can be costly and time consuming. An other method would be to create only one wafer with varying layer thickness in different regions [27]. This may however induce new effects due to the specimen not being homogeneous in the in-plane directions.

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Chapter 4

Annex

4.1 GMSH: 3D mesh of device

This annex is on the GMSH code to generate a 3D mesh of the simplified device.

This mesh has 11 parameters:

- Thickness of the four layers: GaN, SL, AlN and Si.
- Side-lengths of the heater: width and length.
- Maximum size of the elements in the four layers: GaN, SL, AlN and Si.
- Maximum size of the elements in the region underneath the heater, in the layers GaN, SL and AlN.

The maximum size mentioned just above refers to a limit on the size of the elements near a point in the mesh. This constraint propagate through the mesh (i.e. in 3D) between the point with this attribute specified (vertices of the layers and box underneath the heater). There is an interpolation of the maximum element size, in this case it is the default. Please refer to the official GMSH documentation for further information.

Here is the full code for generating the mesh:

```
Mesh.MshFileVersion = 2.2; // Quanscient takes only this version of meshes
Mesh.Algorithm = 6;
```

```
Si_thicc = 100e-6;
AlN_thicc = 175e-9;
SL_thicc = 40e-9 + 30*33e-9;
GaN_thicc = 1.3e-6;
```

```
AlN_bot = Si_thicc;
SL_bot = AlN_bot + AlN_thicc;
GaN_bot = SL_bot + SL_thicc;
GaN_top = GaN_bot + GaN_thicc;
```

```
heater_width = 1e-6;
heater_length = 100e-6;
```

```

Si_len_ratio = 1.5;
Si_spacing = Si_thicc * Si_len_ratio * 2;

Si_length = heater_length + Si_spacing;
Si_width = heater_width + Si_spacing;

Si_size = 100e-6;
AlN_size = 20e-6;
SL_size = 20e-6;
GaN_size = 20e-6;
heater_size = .1e-6;

// #####
// # Points #
// #####

// Si (bot)
Point(1) = {0, 0, 0, Si_size};
Point(2) = {Si_length/2, 0, 0, Si_size};
Point(3) = {Si_length/2, Si_width/2, 0, Si_size};
Point(4) = {0, Si_width/2, 0, Si_size};

// AlN (bot)
Point(5) = {0, 0, AlN_bot, heater_size};
Point(6) = {Si_length/2, 0, AlN_bot, AlN_size};
Point(7) = {Si_length/2, Si_width/2, AlN_bot, AlN_size};
Point(8) = {0, Si_width/2, AlN_bot, AlN_size};

// SL (bot)
Point(9) = {0, 0, SL_bot, heater_size};
Point(10) = {Si_length/2, 0, SL_bot, AlN_size};
Point(11) = {Si_length/2, Si_width/2, SL_bot, AlN_size};
Point(12) = {0, Si_width/2, SL_bot, AlN_size};

// GaN (bot)
Point(13) = {0, 0, GaN_bot, heater_size};
Point(14) = {Si_length/2, 0, GaN_bot, SL_size};
Point(15) = {Si_length/2, Si_width/2, GaN_bot, SL_size};
Point(16) = {0, Si_width/2, GaN_bot, SL_size};

// GaN (top)
Point(17) = {0, 0, GaN_top, heater_size};
Point(18) = {Si_length/2, 0, GaN_top, GaN_size};
Point(19) = {Si_length/2, Si_width/2, GaN_top, GaN_size};
Point(20) = {0, Si_width/2, GaN_top, GaN_size};

// AlN - heater (bot)

```

```

Point(21) = {heater_length/2, 0, AlN_bot, heater_size};
Point(22) = {heater_length/2, heater_width/2, AlN_bot, heater_size};
Point(23) = {0, heater_width/2, AlN_bot, heater_size};

// SL - heater (bot)
Point(24) = {heater_length/2, 0, SL_bot, heater_size};
Point(25) = {heater_length/2, heater_width/2, SL_bot, heater_size};
Point(26) = {0, heater_width/2, SL_bot, heater_size};

// GaN - heater (bot)
Point(27) = {heater_length/2, 0, GaN_bot, heater_size};
Point(28) = {heater_length/2, heater_width/2, GaN_bot, heater_size};
Point(29) = {0, heater_width/2, GaN_bot, heater_size};

// GaN - heater (top)
Point(30) = {heater_length/2, 0, GaN_top, heater_size};
Point(31) = {heater_length/2, heater_width/2, GaN_top, heater_size};
Point(32) = {0, heater_width/2, GaN_top, heater_size};

// #####
// # Lines #
// #####

// Horizontals

// Si (bot)
Line(1) = {1, 2};
Line(2) = {2, 3};
Line(3) = {3, 4};
Line(4) = {4, 1};

// AlN (bot)
Line(5) = {5, 21};
Line(6) = {21, 6};
Line(7) = {6, 7};
Line(8) = {7, 8};
Line(9) = {8, 23};
Line(10) = {23, 5};

Line(11) = {21, 22};
Line(12) = {22, 23};

// SL (bot)
Line(13) = {9, 24};
Line(14) = {24, 10};
Line(15) = {10, 11};
Line(16) = {11, 12};
Line(17) = {12, 26};
Line(18) = {26, 9};

```

```

Line(19) = {24, 25};
Line(20) = {25, 26};

// GaN (bot)
Line(21) = {13, 27};
Line(22) = {27, 14};
Line(23) = {14, 15};
Line(24) = {15, 16};
Line(25) = {16, 29};
Line(26) = {29, 13};

Line(27) = {27, 28};
Line(28) = {28, 29};

// GaN (top)
Line(29) = {17, 30};
Line(30) = {30, 18};
Line(31) = {18, 19};
Line(32) = {19, 20};
Line(33) = {20, 32};
Line(34) = {32, 17};

Line(35) = {30, 31};
Line(36) = {31, 32};

// Verticals

// Si
Line(37) = {1, 5};
Line(38) = {2, 6};
Line(39) = {3, 7};
Line(40) = {4, 8};

// AlN
Line(41) = {5, 9};
Line(42) = {6, 10};
Line(43) = {7, 11};
Line(44) = {8, 12};

Line(45) = {21, 24};
Line(46) = {22, 25};
Line(47) = {23, 26};

// SL
Line(48) = {9, 13};
Line(49) = {10, 14};
Line(50) = {11, 15};
Line(51) = {12, 16};

```

```

Line(52) = {24, 27};
Line(53) = {25, 28};
Line(54) = {26, 29};

// GaN
Line(55) = {13, 17};
Line(56) = {14, 18};
Line(57) = {15, 19};
Line(58) = {16, 20};

Line(59) = {27, 30};
Line(60) = {28, 31};
Line(61) = {29, 32};

// #####
// # Faces #
// #####

// Si
Curve Loop(1) = {1, 2, 3, 4};          Plane Surface(1) = {1}; // bot
Curve Loop(2) = {4, 37, -10, -9, -40}; Plane Surface(2) = {2}; // -x
Curve Loop(3) = {1, 38, -6, -5, -37};   Plane Surface(3) = {3}; // -y
Curve Loop(4) = {2, 39, -7, -38};       Plane Surface(4) = {4}; // +x
Curve Loop(5) = {3, 40, -8, -39};       Plane Surface(5) = {5}; // +y

// AlN
Curve Loop(6) = {6:9, -12, -11};        Plane Surface(6) = {6}; // bot
Curve Loop(7) = {5, 11, 12, 10};        Plane Surface(7) = {7}; // bot small
Curve Loop(8) = {9, 47, -17, -44};      Plane Surface(8) = {8}; // -x
Curve Loop(9) = {10, 41, -18, -47};     Plane Surface(9) = {9}; // -x small
Curve Loop(10) = {6, 42, -14, -45};     Plane Surface(10) = {10}; // -y
Curve Loop(11) = {5, 45, -13, -41};     Plane Surface(11) = {11}; // -y small
Curve Loop(12) = {7, 43, -15, -42};     Plane Surface(12) = {12}; // +x
Curve Loop(13) = {8, 44, -16, -43};     Plane Surface(13) = {13}; // +y

// SL
Curve Loop(14) = {14:17, -20, -19};     Plane Surface(14) = {14}; // bot
Curve Loop(15) = {13, 19, 20, 18};     Plane Surface(15) = {15}; // bot small
Curve Loop(16) = {17, 54, -25, -51};    Plane Surface(16) = {16}; // -x
Curve Loop(17) = {18, 48, -26, -54};    Plane Surface(17) = {17}; // -x small
Curve Loop(18) = {14, 49, -22, -52};    Plane Surface(18) = {18}; // -y
Curve Loop(19) = {13, 52, -21, -48};    Plane Surface(19) = {19}; // -y small
Curve Loop(20) = {15, 50, -23, -49};    Plane Surface(20) = {20}; // +x
Curve Loop(21) = {16, 51, -24, -50};    Plane Surface(21) = {21}; // +y

// GaN
Curve Loop(22) = {22:25, -28, -27};     Plane Surface(22) = {22}; // bot
Curve Loop(23) = {21, 27, 28, 26};     Plane Surface(23) = {23}; // bot small

```

```

Curve Loop(24) = {25, 61, -33, -58}; Plane Surface(24) = {24}; // -x
Curve Loop(25) = {26, 55, -34, -61}; Plane Surface(25) = {25}; // -x small
Curve Loop(26) = {22, 56, -30, -59}; Plane Surface(26) = {26}; // -y
Curve Loop(27) = {21, 59, -29, -55}; Plane Surface(27) = {27}; // -y small
Curve Loop(28) = {23, 57, -31, -56}; Plane Surface(28) = {28}; // +x
Curve Loop(29) = {24, 58, -32, -57}; Plane Surface(29) = {29}; // +y

Curve Loop(30) = {30:33, -36, -35}; Plane Surface(30) = {30}; // top
Curve Loop(31) = {29, 35, 36, 34}; Plane Surface(31) = {31}; // top small

// #####
// # Volumes #
// #####

Surface Loop(1) = {1:7}; Volume(1) = {1};
Surface Loop(2) = {6:15}; Volume(2) = {2};
Surface Loop(3) = {14:23}; Volume(3) = {3};
Surface Loop(4) = {22:31}; Volume(4) = {4};

// #####
// # Define groups #
// #####

Physical Volume("Si layer") = {1};
Physical Volume("AlN layer") = {2};
Physical Volume("SL layer") = {3};
Physical Volume("GaN layer") = {4};

Physical Volume("Heat targets") = {1:4};
Physical Volume("All") = {1:4};

Physical Surface("Heater surface") = {31};
Physical Surface("Chuck") = {1};

Physical Volume("Layers", 10) = {2:4};

Physical Curve("Si line") = {37};
Physical Curve("AlN line") = {41};
Physical Curve("SL line") = {48};
Physical Curve("GaN line") = {55};

Mesh 2;
Mesh 3;
OptimizeMesh "Gmsh"; // optimize mesh as there's a high change
                      // of ill-shaped tets being still there

Save "meshes/main.msh";
Printf("Done meshing!");

```

4.2 Heater resistance values for Si samples

This annex is on the value of the resistance of the heaters on the Si samples measured for the extraction of thermal conductivity via the 3-omega method.

width [μm]	B	C	D	E
5	2985	2870	2670	
10	1570	1593	1430	
25				684
50				347

Table 4.1: Values of the resistance of the heater for the silicon samples. Values are in Ω .

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