Declaration of Committee

Name: Kurtis J. Raymond

Degree: Master of Applied Science


Committee:

Chair: Jie Liang
Professor, Engineering Science

Andrew Rawicz
Supervisor
Professor, Engineering Science

Fabrice Retière
Committee Member
Adjunct Professor, Physics

Shawn Sederberg
Examiner
Assistant Professor, Engineering Science
Abstract

An experimental setup was developed for analyzing the secondary photons produced by the Geiger mode avalanches utilized by Silicon Photomultipliers (SiPMs). The spectrum of these secondary photons previously has never been measured at the normal operating ranges of SiPMs. While secondary photons have an impact on the performance of SiPM themselves, they can also escape their source SiPM and trigger additional signals in other SiPMs. For this reason, secondary emission is of great importance of large photosensitive detectors. This work characterizes two SiPM devices of interest for the next Enriched Xenon Observatory (nEXO) double beta decay experiment: the FBK-VUV-HD3 and HPK-VUV4. The measurements reported in this work are intended to be used in a Monte-Carlo simulation of a smaller scale liquid xenon detector system called LoLX for understanding the impact of secondary emission in a larger detector system such as nEXO.

Keywords: SiPM; Single Photon Sensors; Secondary Emission; Single Photon Avalanche Diodes
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List of Acronyms

DAQ Data AQuisition System.

FBK Fondazione Bruno Kessler.

HPK Hamamatsu Photonics.

LAr Liquid Argon.

LXe Liquid Xenon.

MIEL Microscope for the Injection and Emission of Light.

NA Numerical Aperture.

PDC Photon-to-Digital Converter.

PDE Photon Detection Efficiency.

SiPM Silicon Photomultiplier.

SPAD Single Photon Avalanche Diode.

VERA Vacuum Emission Reflection Absorption.
Chapter 1

Introduction

Detectors are the limit of technological development. They define and verify our understanding of physical phenomena, aid in diagnostics, and allow for further developments technological beyond themselves. Detectors additionally form the cornerstone of experimental physics, which is a constant quest for the direct detection of some phenomena. In the case of dark matter, there is a lot of support for the existence of something, including where it is spatially located, but there has never been an observed case of how it interacts with normal matter, and its signature has never directly been manifested. However, this quest for direct observation has lead to the development of a unique set of detector systems for which requirements are highly specialized.

For the next generation of photon detection, the conventional photomultiplier tube is no longer satisfactory. New particle physics experiments, which need to detect single photon level signals, require detector systems with a huge amount of sensitive mass, low radioactive background, and high stability. The current development of Vacuum Ultraviolet (VUV) Silicon Photomultiplier (SiPM) devices are trending to satisfy these requirements over previous photo-detectors.

The work presented here is one aspect into the development of SiPMs. The avalanche process which is the main detection mechanism of an SiPM generates a large quantity of “hot” charge carriers which may produce secondary photons. The impact of this can be measured on the device level as an excess signal generated, with both a prompt and delayed component. Methods to mitigate the secondary photons have been implemented on a number of SiPM devices with great success, but fails to consider the implication of these secondary photons on a wider system involving multiple SiPMs, or changes to the optical structure of the SiPM itself. A greater understanding of these byproduct photons, including spectral composition and absolute production, can be used to guide simulations on both the device and system level to understand their true impact on developing devices and detector systems.

Two devices were selected as initial subjects for measuring these byproduct photons, the FBK-VUV-HD3 and HPK-VUV4 device. The two devices were designed and developed by
different companies and labs, and feature different internal structures. The exact structure are often trade secrets or proprietary. Effort was made to use and develop simple models, which are applicable to future device developments. These two devices are candidate devices for the next Enriched Xenon Observatory (nEXO) which is a ton-scale double-beta decay detector. These devices represent the state of the art SiPMs for VUV detection.

These devices are also utilized in the Light only Liquid Xenon (LoLX) detector, which is a small scale LXe detector system to serve as a test bed for SiPMs intended to be used in larger LXe detector systems. Phase one of LoLX utilized the HPK-VUV4 SiPMs, which will be introduced later. Measurements performed and models developed in this work are to be utilized in a Monte-Carlo simulation of the phase one LoLX detector system to demonstrate a complete understanding of the impact of secondary photons on a larger detector system.

A large component of this work was developing the Microscope for the Injection and Emission of Light (MIEL). As its name suggests, it utilizes a laser to stimulate single SPADs, and is capable of measuring the secondary emission of light from SiPMs simultaneously with stimulation. Care was taken to ensure that the instrument was calibrated to measure the absolute light observed so that its results could be used to calculate the impact of secondary photons on a number of performance parameters relevant to devices and detectors. The MIEL setup is described and its operation outlined in Chapter 2.

Extrapolating to the light produced at the source from the measurements obtained using MIEL required extensive optical surface modelling. Additional extrapolation is performed to find the total light emitted by the SiPM in various media, which are instrumental to understanding the impact of secondary light on a wider detector system. To verify the optical surface modelling, a comparison between ellipsometry measurements using the Vacuum Efficiency, Reflectivity, and Absorption (VERA) setup is made. The theory and verification work is contained in Chapter 3.

The data analysis to take the raw image data produce by MIEL’s cryogenic camera, and SiPM signal waveforms, from the MIEL setup into a emission spectrum is contained in Chapter 4. The extensive modelling calculated in the previous chapter is used to inspect what shape the emission spectra could take in various operating conditions such as in air or liquid xenon detector systems.

Emphasis has been placed on developing clear and simple models which are applicable to the development of SiPM devices. This strategy is emphasized due to the lack of information provided by SiPM manufacturer’s on the internal structure of SiPM devices, variation from batch to batch of the same SiPM devices, and intuitive nature of the models constructed.

The remaining sections in this chapter briefly discuss the history of SiPM development from the inception of avalanche breakdown in P-N junction. It is followed by a discussion of the impact of the secondary emission from avalanche breakdown on devices, and how this work can aid in mitigating the effect of secondary emission on SiPMs and detector systems which use them.
1.1 Silicon Based Single Photon Sensors

The first demonstration that electron multiplication occurs under the injection of charge carriers into a highly reversed biased germanium \( p - n \) junction was in 1953 [25]. This principle relied on a large electric field capable of energizing electrons to energies capable of ionizing other atoms, which is so-called impact ionization. The first theory of electron multiplication was put forth in 1954, assuming that the electron multiplication was similar to gas discharges [39].

In 1966 it was proposed to use impact ionization in a photodiode to proportionally increase the signal to noise ratio in detector systems where the noise is dominated by sources external to the photodiode [24]. The proposed detector specifically excluded using excessive multiplication rates, of which current generation SiPM are based on.

The first detector concept, although still labelled as an Avalanche Photodiode (APD), which is most similar to modern day SPAD was proposed in 2000 [34], which utilized the Geiger mode breakdown to detect single photons. The first published description of the Silicon Photomultiplier (SiPM) was in 2002 [6] using a grid of quenched avalanche photodiodes [8] developed in 1996. Since this inception, SiPMs have enjoyed a continued development due to their attractiveness in a range of options and as an alternative to conventional photomultiplier tubes.

SiPMs are composed of a tightly packed array of single photon avalanche diodes (SPADs). The structure of SPADs are \( p - n \) junctions designed to have a sufficiently high electric field above some operational breakdown voltage, \( V_{br} \), to sustain impact ionization. An avalanching SPAD forms a microplasma within the \( p - n \) junction and a large number of charge carriers are generated, which rapidly causes the \( p - n \) junction to conduct. A quenching resistor \( R_q \) is placed in series with the junction to induce a voltage drop across the active avalanching \( p - n \) junction and promptly neutralize the microplasma. After some recharge time, \( \tau_r \), the depletion region within the \( p - n \) junction is reformed and the SPAD is ready to fire again. An effective circuit model of a SPAD is shown in Figure 1.2, and the equivalent circuit parameters are shown in Table 1.1. A pictorial side view of a SPAD is shown in Figure 1.1a, and the top view of an SiPM is shown in Figure 1.1b.

The avalanching SPAD generates a consistent number of charge carriers at each operating voltage, irrespective of the number of initial number of charge carriers present.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Aprox Value</th>
<th>Full Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>( R_q )</td>
<td>( \sim 1M\Omega )</td>
<td>Quenching Resistor</td>
</tr>
<tr>
<td>( C_q )</td>
<td></td>
<td>Parasitic Capacitance</td>
</tr>
<tr>
<td>( R_d )</td>
<td></td>
<td>Electrical Resistance</td>
</tr>
<tr>
<td>( C_d )</td>
<td>( \sim fF )</td>
<td>Single Cell Capacitance</td>
</tr>
<tr>
<td>( V_{bd} )</td>
<td>20-50V</td>
<td>Breakdown Voltage</td>
</tr>
</tbody>
</table>

Table 1.1: Equivalent circuit parameters of an SiPM device.
Proportionality in the incoming light signal is achieved by having a large number of SPADs on a single SiPM and counting the number of SPADs which have fired simultaneously. The output of the SiPM can then be classified as the number of $n$-photoelectrons ($n$PE). The inherent gain within the SPAD is given by $G_{PE}$, and it is related to the single photoelectron (PE) charge, $Q_{PE}$, and the electron charge $q_E$,

$$G_{PE} = \frac{Q_{PE}}{q_E}$$

(1.1)

The single PE charge is directly proportional to the operational over-voltage, $V_{ov}$, through the single cell capacitance $C_D$. 

---

Figure 1.1: Side (a) and Top view (b) of an pictorial representation of an blue sensitive $p$-on-$n$ analog SiPM device. The light region bounded by the red line is high field region where the impact ionization occurs. The trench offers an optical isolation between different SPADs on the same device, and are often accompanied by other nuisance mitigation structures.

Figure 1.2: Equivalent circuit model of a SPAD the circuit parameters are contained in Tab. 1.1. Reprinted from Ref.[1].
Figure 1.3: A single photo-electron pulse from a FBK-VUV-HD3 SiPM. The leading edge and falling edge are clearly visible. The time constant of the rising edge depends on the formation of the avalanche in the SPAD, and the falling edge depends on the resistances within the device and external electronics.

\[ Q_{PE} = C_d \times (V - V_{br}) \]  
\[ = C_d \times V_{ov} \]  

Rise time, \( \tau_r \), of a SiPM is related through the \( C_D \) and the parasitic quenching capacitance, \( C_q \), the quenching resistance, \( R_q \), and the diode resistance, \( R_d \), [7],

\[ \tau_r = (C_d + C_q) \times (R_q || R_d) \]  

The recharge time is related through the inherent resistance within the SPAD, and the total capacitance within the SPAD,

\[ \tau_{recharge} = R_d \times (C_d + C_q) \]  

One note will be made that the external amplifier system may have some impact on the recharge as well.

An amplified and digitized signal produced from a FBK-VUV-HD3 SiPM device is shown in Figure 1.3. A clear fast rise time and slow decay time is apparent.

The probability that an impinging photon is detected by the SiPM is known as the Photon Detection Efficiency (PDE). SiPMs are often designed with detecting photons of specific wavelengths. For instance, a common particle detection scheme consists of coupling
an SiPM with a material which emits light when energy is deposited into it. A robust scintillator is BC-400, which is known to emit 408 nm light under stimulation, creates the need for SiPMs on the market which are designed to detect light from 400 nm to 430 nm. Additionally, a great effort has been put into developing SiPMs capable of detecting light in the vacuum ultraviolet wavelengths (VUV) due to the development of cryogenic noble scintillators. Specially designed devices were developed to limit the insensitive boundary of the $p – n$ junction where high energy VUV photons are most likely to be absorbed.

A simplified description of the PDE is given by Ref. [41],

$$PDE = FF \cdot \epsilon(\lambda) \cdot T_P(V, \lambda)$$

Where FF is the fill factor of the device,

$$FF = \frac{\text{Sensitive Area}}{\text{Total Area}}$$

And $\epsilon(\lambda)$ is the quantum efficiency of the device, and $T_P(V, \lambda)$ is the probability of triggering an avalanche given the impinging photon created an electron-hole pair. The PDE of an SiPM can also be separated into two parts, the optical portion and the internal PDE. Both of these portions will be discussed in Section 3.2, where extensive modelling is performed.

## 1.2 SiPM Luminescence

The majority of the “hot” charge carriers generated during an avalanching SPAD will return to a normal state through non-radiative means, but a small number of electrons will decay by emitting light. The secondary photons produced in SiPM are the cause of several nuisance phenomena present in SiPMs: internal cross-talk, external-cross-talk and optical produced after-pulsing[5]. This section will discuss their origins and impact on the device level, and system level. The main three processes of optical cross-talk described here are shown in Figure 1.4.

Internal cross-talk occurs when a photon from one SPAD travels to the vicinity of another SPAD, generates an $e – h$ pair, and one of the charge carriers of the pair travels to the sensitive region of the SPAD. The time scale of internal cross-talk heavily depends on where the $e – h$ pair is generated.

Direct cross-talk results when the cross-talk signal is superimposed onto the original signal. This leads to a signal which is larger than what is initially created. Conversely delayed cross-talk produces a pulse which is not superimposed onto the original signal, and can be distinguished from the original signal by a separate, but delayed, pulse. When the original SPAD has fully recharged, it is difficult to distinguish between delayed cross-talk and any and all forms of after-pulsing, which will be discussed later.
Figure 1.4: Mechanisms of internal/external/delayed optical phenomena as shown for an $n – on – p$ device sensitive to electrons in the bulk. Reprinted from Ref. [31]. In prompt or direct cross-talk, the secondary photon is produced in the source SPAD and directly travels either in or nearby the avalanche region of a nearby SPAD. Delayed cross-talk is similar, but the electron is produced in the bulk, and the signal is delayed by the travel time of the electron. And lastly, external cross-talk is considered when an external optical interface is included, and the secondary photon reflects off this interface to produce prompt cross-talk.

Several methods exist for mitigating the effects of direct cross-talk. Optically semi-transparent or opaque materials can be filled into “trenches” between SPADs to block light from travelling directly from SPAD to SPAD. SiPMs designed for detecting UV wavelengths are only interested in photo-electrons which come from the front of the detector, and thus can employ doping schemes to mitigate holes generated in the bulk from secondary photons.

External cross-talk can be broken down to two situations. The secondary photon can leave the SPAD, and reflect back from either surface structures or external optical structures [31, 17] and enter the same SiPM again and trigger another SPAD. The surface structure of the same SiPM device can change depending on what detector system is placed in (ie, additional protective windows, filters, different mediums of refraction LXe, LAr), which makes characterizing the impact of external cross-talk difficult on the device level. The secondary photon can also leave the SiPM entirely and become detected in another SiPM visible to it either directly or through reflection [26]. Thus, systems which utilize a large photo-sensitive area, or a large number of SiPMs, are more susceptible to a degradation in performance due to external cross-talk.

Optical after-pulsing occurs when a secondary photon creates an $e – h$ pair deep in the bulk, which eventually travels to the same SPAD which it subsequently triggers. The signal produced is identical to after-pulsing by charges which become trapped in the lattice structure and subsequently become released to trigger the same SPAD again.

For any of the above proposed mechanisms, the impact that secondary photons depends on the amount of secondary photons produced each avalanche, and the wavelength of that light. Previous characterizations of light produced from avalanches in silicon indicate that very few of the photons are produced with short wavelengths, while the majority are in the
visible (VIS) and near-infrared (NIR) [23, 27]. This implies that SiPMs designed to detect NIR light are potentially impacted more, as the secondary photons will produce charge carriers deep in the bulk similar to the signal.

If we consider only the average behaviour of the SiPM, a simplified equation can be written which aids in understanding the mechanism of internal cross-talk. We define $n_\gamma(V_{oV}) = G(V_{oV}) \cdot \eta_{ph}(V_{oV})$ to be the number of photons produced at the source at a voltage above the breakdown, $V_{oV}$, for probability that a charge carrier involved in the avalanche can generate a secondary photon, $\eta_{ph}$, which may nor may not be field or operating voltage dependent. And $G(V_{oV})$ is the gain, or the number of charge carriers generated in an avalanche. If we assume that each photon has a potential chance of causing an avalanche in another SPAD, and the number of photons produced at the source is large, $P_{ICT} = 1 - (1 - \epsilon_{ICT} \cdot P_{Avalanche}(V_{oV}))^{n_\gamma(V_{oV})}$ (1.6)

The $\epsilon_{ICT}$ parameters is dependent on the internal geometry of the device, and the wavelength of light produced during the avalanche, and can be considered as the transport from one SPAD to another. The $P_{Avalanche}(V_{oV})$ parameter is the probability of a charge carrier causing an avalanche, and it is an average behaviour of hole and electron driven avalanches generated at points within and around the active region. This indicates that the probability of causing another avalanche on the same SiPM is directly related to the number of photons produced at the source of the avalanche.

Similar to internal cross-talk, external cross-talk can be treated in a similar way. The transport and detection efficiency parameters are no-longer internal, and deal with exter-
nally measured responses. Again, for a large number of photons produced at the source, we can write,

\[ P_{eCT} = 1 - (1 - P_t \cdot \text{PDE}(V_{oV}))^{(\eta_{esc} - n_s(V_{oV}))} \] (1.7)

The \( \eta_{esc} \) parameter is the probability that a photon generated will escape the SiPM entirely. \( P_t \) is the probability that an escaping photon travels to another photo-site, and \( \text{PDE}(V_{oV}) \) is the photon detection efficiency averaged over the angles seen by that detector.

The effect of external cross-talk is often overlooked during the design of a device. Designers will often introduce optical blocking materials between SPADs, which allow devices to mitigate internal cross-talk and run at higher operating voltages. However, these additional photons generated at higher over-voltages do have an impact on the external cross-talk probability. Previous publications which measure the emission with respect to the charge carriers within the avalanche place the intensity of emission at an order of \( 1 \times 10^{-5} \) photons/e- [23, 27], which indicates that a larger gain will imply more secondary photons produced.

An illustrative example of external cross-talk is to consider the case of a large detector system. The process of external cross-talk for both the production and detection will be assumed to be Poissonian for simplicity, and this assumption may hold in a large detector system due to the large number of available photo sites. This example will be returned to in the conclusion, but using the measurements obtained in this work, however it is illustrative to set up the brief mathematical framework in context of this work.

Consider a SPAD on an SiPM which avalanches and emits an average of \( n_s \) secondary photons. These photons are then transported to another SiPM where they may be absorbed with some average probability, \( P_a \). In reality, the detection efficiency is heavily dependent on the optical surface structure, the wavelength of the light produced, angle of emission, and position of the source and target SiPMs in the detector system. We let \( \lambda = n_s P_a \) be the Poissonian parameter, and state that \( \lambda \) is the mean number of additional avalanches which follows a single avalanche. Thus to obtain meaningful information out of the detector system, we set the bound \( |\lambda| < 1 \). In the behaviour of a real detector system where \( \lambda > 1 \), the result is certainly catastrophic where all the SiPMs in a system will fire and all information is lost. Since each secondary SiPM which avalanches due to the first initial avalanche also produces additional photons, the process will continue until no more SiPMs avalanche. This behaviour can be modelled by a geometric series (See Eq. 3.28), and the additional
avalanches can be considered to be some kind of gain parameter $g$,

$$N = n \cdot g = n \cdot (1 + \lambda + \lambda^2 + \cdots)$$  \hspace{1cm} (1.8)

$$= n \sum_{i=0}^{\infty} \lambda^n$$  \hspace{1cm} (1.9)

$$= n \cdot \frac{1}{1 - \lambda}$$  \hspace{1cm} (1.10)

Here $n$ is the initial number of photons produced by a signal, and the previous restriction of $|\lambda| < 1$ preserves the geometric series assumption. This signal can either be a scintillation signal, for example, or from a spontaneous dark avalanche. The latter of which has a heavy implication for detecting low level signals, such as the case with dark matter detection systems.

The gain can also be translated into the mean number of additional avalanches which will allow a comparison to be made to the internal cross-talk figures of merit called the mean number of additional prompt avalanches,

$$N_{apa} = g - 1$$  \hspace{1cm} (1.11)

To avoid complicating the narrative, despite the small value of $\lambda$, the normal approximation of the Poissonian distribution will be applied to show the loss in energy resolution of a detector system due to the statistical fluctuations of secondary cross-talk. This can be done by inspecting the standard deviation of the gain term,

$$\delta g = \frac{\sqrt{\lambda}}{1 - \lambda} = \sqrt{\lambda} \cdot g$$  \hspace{1cm} (1.12)

This term grows similarly as the normal standard deviation of a Poissonian until it begins to grow faster ($\sim 0.02 = \lambda$). Thus, the whole detector system has a signal-to-noise ratio,

$$\text{SNR} = \frac{1}{\sqrt{1/n + \lambda}}$$  \hspace{1cm} (1.13)

This equation reduces to the standard Poissonian SNR when $\lambda = 0$, but degrades the SNR of a detector system by roughly half when $\lambda = 0.2$ when compared to when $\lambda = 0$ (normal Poissonian), which shows the impact of external cross-talk could potentially be huge. This is especially important as the photon detection efficiency of most SiPM devices are between 0.2 to 0.6, and so if only a handful of photons are produced in the relevant wavelength ranges, then the values for $\lambda$ stated here are not so unrealistic. However, as shown later,
the majority of light produced is in the NIR region, which blue-sensitive SiPMs have lower detection efficiencies for.

Secondary photons also impact the design of devices which are not SiPMs, but nonetheless rely on the use of Geiger mode avalanches. An example of this is the Array of Saturated Gain Avalanche Diode (ASGAD) detector concept for the detection of charge particles, which relies on correlated avalanches between different cells to identify and provide timing for charge particles, as an alternative to CCD based charged particle detectors. In this concept, secondary photons are a nuisance which can potentially heavily degrade the concept of this detector, as the secondary photons can travel and generate $e^–h$ pairs deep in the bulk, which can mimic the charge generated along a track left by an ionizing particle. For additional details see Ref. [32]

1.2.1 Secondary Light Production Mechanisms

The first light emission observed from a silicon $p–n$ junction under a high reverse bias was reported in Ref. [29] in 1955. The light emission coincided with a sharp increase in reverse bias current. They attempted to correlate the light emission with the so-called electron-multiplication reported in Ref. [25] but stated only inconclusive results, although they asserted that the most likely explanation was due to the breakdown in Silicon. Under this assumption, they provided a spectrum of the light generated within the junction, which is shown in Fig. 1.6. We now know this light is a consequence of avalanche breakdown, which is used in SPADs as the mechanism to detect single photons. Thus as a consequence of the light detection mechanism, secondary light is produced. This section seeks to describe the mechanism of light production in a silicon $p–n$ junction.

Since the measurement reported in 1955, a number of papers have been published measuring and characterizing the source of light from $p–n$ junctions in avalanche breakdown [40, 18, 36, 9]. A the most recent work which proposes a possible number of emission mechanisms in $p–n$ junctions is in Ref. [3]. A figure showing the various emission mechanisms pictorially is shown in Figure 1.7.

1.3 Selection of SiPM devices for testing

The SiPM devices chosen for this work are relevant to the next Enriched Xenon Observatory (nEXO). The nEXO experiment is a continuation of the development of the EXO-200 detector, which uses Liquid $^{136}$Xe (LXe) as its detection media. Along with utilizing LXe, nEXO has an electrode and an anode to operate as a time projection chamber (TPC) for charge collection, and providing spacial sensitivity. Liquid Xenon is a cryogenic scintillator which produces 178 nm photons under stimulation, which poses a unique requirement on the photo detector system.
Figure 1.6: Light emitted from a silicon $p-n$ junction operated in the breakdown region. The spectrum has been corrected for as if the light was produced from the $p-n$ junction. Taken from Ref. [29].

Figure 1.7: Band diagram models showing the various proposed emission mechanism of Ref. [3]. Provided by Pietro Giampa.
Table 1.2: Parameters of devices characterized in this work [15].

<table>
<thead>
<tr>
<th>Parameter</th>
<th>FBK-VUV-HD3</th>
<th>HPK VUV4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total Area</td>
<td>6×6mm²</td>
<td>3×3mm²</td>
</tr>
<tr>
<td>Fill Factor</td>
<td>80%</td>
<td>60%</td>
</tr>
<tr>
<td>SPAD Pitch</td>
<td>35 × 35 µm²</td>
<td>50 × 50 µm²</td>
</tr>
<tr>
<td>SPAD capacitance (fF)</td>
<td>90 ± 5</td>
<td>101 ± 7</td>
</tr>
</tbody>
</table>

The nEXO experiment is specifically designed to look for the signature signal of a theoretical decay mode of neutrinoless double beta decay \((0νββ)\), and previous iterations have bounded the half-life of this elusive decay mode to \(2.16 ± 0.06 \times 10^{25}\) yrs at a 90% confidence interval [4]. To prove the existence of neutrinoless double beta decay is a delicate task that requires a great understanding of the response of the detector system, and the signal background.

The two candidate SiPM devices intended to make up the photo-sensitive area of nEXO, as shown in Figure 1.8, are the devices designed by Fondazione Bruno Kessler (FBK) and Hamamatsu Photonics K.K. (HPK) specifically designed for detecting Vacuum Ultraviolet photons. The third generation device from FBK (FBK VUV-HD3) and the forth generation HPK device (HPK VUV4) have been extensively tested for use in nEXO [15]. A summary of device parameters is shown in Table 1.2. However, these devices have only been independently tested in isolation. To understand the impact of external cross-talk of these devices is one aspect of the work in this thesis.

While these two device are the study of this work, the intention is for the development of a system which can perform characterizations on similar SiPM devices from other manufactures. The characterization of these devices is also a stepping stone to understand the production mechanism at the source of these photons. This will lead to a complete set of tools to allow future SiPMs to be designed with the impact of cross-talk fully considered, as well as allowing for the design impact of external cross-talk on future detector systems.

Complimentary to this work is the Light Only Liquid Xenon (LoLX) detector. This is a smaller analogous detector system to the nEXO experiment which utilizes the same SiPM devices as nEXO. A side section showing the similarity to the nEXO detector system is shown in Figure 1.9. Spectral measurements, and optical modelling of the SiPM’s surface layers are used in a Monte-Carlo simulation of the LoLX detector system. For additional details for the LoLX system, see Ref. [12].

1.4 Development of Future SiPM Devices and SiPM based detectors

As mentioned previously, this work aids in the development of future detectors and devices by three avenues. Knowing the structure of photon production at the source allows for
Figure 1.8: Cross-section of the nEXO time projection chamber (TPC). The blue portion on the interior of the cylinder is the photo-sensitive area of the nEXO experiment. The cylinder has a diameter of 1.5 m, and the two ends are capped by reflective surfaces. Reprinted from Ref. [2].

Figure 1.9: Cross-section of the phase one LoLX detector. Roughly 2 in in diameter. The light grey squares show the location of single SiPMs arranged in a hexagonal shape. The LoLX detector is an excellent test bed for the impact of external cross-talk on LXe detector systems due to the large number of unique angles, and similarity to what a practical LXe detector would be. Courtesy of David Gallacher.
Figure 1.10: Context surrounding the measurements performed in the MIEL setup. The boxes in green show the bulk of the work of this thesis. QLADS is a software package for the simulation photon and charge transport. The ultimate goal of this ecosystem is the continued development of devices using Geiger mode avalanches to detect single photons, and the development of detector systems which utilize those detectors. MIEL and VERA are both SiPM characterization systems which are discussed in Sec. 2 and Sec. 3.2.1. The initial optical modelling and SiPM surface modelling is outlined in Sec. 3. The Light emission measurements are described in Sec. 4.6.

accurate modelling of both absolute photon emission from SiPM devices, and the impact of internal cross-talk on those devices. To use either of these results require accurate carrier transport and photon transport within a medium such as Silicon. This work aids in this understanding by tackling a subset of the requirements to inform the design of new devices and detectors, as shown in Figure 1.10. An example of a new detector design which could be aided with the measurements performed in this work is the challenge of making a backside illuminated (BSI) SiPM.

A BSI SiPM is analogous to the conventional BSI CMOS sensors [28, 21]. The production of BSI SiPMs would have a number of advantages. In BSI design, the surface structure is entirely independent from the internal device design. The backside surface structure can be constructed depending on the desired detection wavelength, such as VUV-detection (p-on-n), or near infrared (large bulk n-on-p). In a BSI configuration there is no mechanical interference from electrical contacts which allows for a stronger coupling to the outside media. This advantage also has better control over the surface structure, and decoupling the design of the avalanche region with the surface structure. An example of this is the development of black SiPMs (b-SiPMs) which may require BSI technology[22, 37, 38] to achieve both reliable SiPM performance, and a PDE near or above unity.
Similar to BSI CMOS sensors, BSI also allows for direct readout using custom ASICs. This unlocks the ability to have dense sets of digital SiPMs, or custom outputs which require no external analog electronics, or 3D integration.

However, the development of BSI-SiPMs generally have a number of drawbacks relating to the production of secondary photons. BSI sensors typically have a large bulk, which leads to increased dark count rate (especially for p-on-n devices), and increased optical cross-talk. FBK has a first demonstrator BSI-SiPM for IR detection [30].
Chapter 2

The Microscope for the Injection and Emission of Light

2.1 Introduction

This section is used to provide a potential student or experimental user with the basic knowledge of the subsystems involved in the microscope for the injection and emission (MIEL).

This section discusses the use of a microscope to simultaneously stimulate and measure the emission of a single SPAD on a SiPM. An example of this is shown in Figure ?? . MIEL consists of a cooled X-Y stage, confocal microscope, stimulation laser, and a spectrometer.

2.1.1 Confocal Microscope System

A basic schematic of the confocal microscope system is shown in Figure 2.2. An interior photo of the vacuum chamber is shown in Figure 2.3, and the difficult to see structure is shown in Figure 2.4.

A list of possible microscope objectives are contained in Table 2.1. The choice of which microscope objective depends on several factors, with the main choice being magnification. The 4x objectives allow for a large portion of the SiPM to be visible. The 20x objective allows for a SPAD a large portion of its neighbours to be visible, and allows for a good compromise between stimulation spot size and SPAD size. The 40x and 50x objectives are specifically chosen for looking at a SPAD and its nearest neighbours, or sub-SPAD effects.

A photo of the MIEL setup after being installed on the optical table in January 2022 is shown in Figure 2.5. The current state of the MIEL setup is shown in Figure 2.6. While the setup looks similar, a number of upgrades have been performed,

- The LN2 dewar has been placed higher up to improve cooling performance. Previously, when the top of the dewar was inline with the upper cold plate, the setup struggled to maintain a temperatures below -110°C. By placing the dewar higher, the MIEL setup
Figure 2.1: Comparison with reflected light image (a) with emission map (b) of a FBK-VUV-HD3 sample. The light from (b) is avalanches due to the main central SPAD and cross-talk to neighbouring SPADs. Image (a) shows a black-body light source focused onto the main SPAD. In image (b) the light source has been exchanged with a stimulation laser and is filtered out before being recorded.

<table>
<thead>
<tr>
<th>Objective</th>
<th>Full Name</th>
<th>Magnification</th>
<th>Numerical Aperture</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>LCPLN20XIR</td>
<td></td>
<td>20x</td>
<td>0.45</td>
<td>NIR</td>
</tr>
<tr>
<td>LmplFLN20X</td>
<td>LmplanFL N</td>
<td>20x</td>
<td>0.40</td>
<td>VIS</td>
</tr>
<tr>
<td>LMPPLFLN10X</td>
<td></td>
<td>10x</td>
<td></td>
<td>VIS</td>
</tr>
<tr>
<td>LCPLN50XIR</td>
<td>Lmplan N</td>
<td>50x</td>
<td>0.65</td>
<td>NIR</td>
</tr>
<tr>
<td>–</td>
<td>Pike Tech</td>
<td>40x</td>
<td>0.78</td>
<td>Reflective, VIS-NIR</td>
</tr>
</tbody>
</table>

Table 2.1: List of Microscope Objectives available in the MIEL setup. The objectives are noted if they are to be used for near-infrared (NIR) or visible (VIS) wavelength ranges.

is able to obtain temperatures ranging from -173°C to -187°C, depending on the heat load inside the vacuum chamber.

- Additional flanges and connections were installed to support the development of the Photon-to-Digital (PDC) converter. This device is similar to an analog SPAD, but it is actively controlled to quench the avalanching diode. Compared to an analog SPAD, a control board is interfaced with a daughter board located in vacuum.

### 2.1.2 Vibration Dampening

Due to the high magnification and high center of mass, the MIEL setup is sensitive to vibrations. Previously, the setup was mounted on a table top, but with the added vacuum chamber, vibration were apparent on any exposures. As such, the setup is mounted on an optical table with isolating legs to minimize vibration induced from the room. The cryogenic
Figure 2.2: The main components of the optical path inside MIEL. The blue beam shows the light which travels from a stimulation laser light source, reflects off a specifically chosen dichroic filter. The light is then focused onto a single SPAD. After the SPAD avalanches, the light labelled as red is from the secondary emission. This light is refocused by the objective, transmits through the dichroic and emission filter, of which it is focused into the HRS-300 spectrograph. The BaF$_2$ cube is for optionally illuminating the sample for positioning.
Figure 2.3: Interior photo of the MIEL vacuum chamber. The SiPM is mounted on the bottom of the X-Y stage, and the Tri-X cable (left side) connects the SiPM to the feedthrough to read the detectors response out of the chamber. The copper braided thermal connections are visible descending from the top of the chamber. The blue cabling is for resistance temperature detectors (RTDs) located on each corner of the stage. The red cabling is connected to two 20W heaters.
Figure 2.4: Side profile view of Figure 2.3 in Computer Aided Design (CAD) showing the individual parts of the vacuum chamber. The feed-throughs which connect the LN2 lines to the cold stage are on the left side out of view. The microscope objective looks through a thick sapphire window onto the SiPM position. Optional z-height adjustment is performed using a micrometer located on top of the vacuum chamber.
Figure 2.5: The MIEL setup installed on an optical table in January 2022

Figure 2.6: The MIEL setup in November 2023
connection to the suction pump is decoupled by using silicon tubing. The turbomolecular pump, which maintains the vacuum system, is decoupled from the backing pump. The former of which does not introduce any observable vibration, and any high frequency vibrations emitted are easily filtered by the sheet of sorbothane it is mounted upon.

To evaluate the effect of the optical table, the power spectrum was obtained using a digital signal analyzer and a Dytran3100D24T accelerometer. The optical table resulted in a reduction of nearly 100x across the entire spectrum, with a reduction of 1000x in the less than 100 Hz frequency range.

2.1.3 Vacuum System

A vacuum system consists of a sealed container and pumping system. The sealed container is pumped until only residual gasses remain. This section will briefly discuss the vacuum system for MIEL and its design.

At low pressures, the gas molecules hardly interact with each other, and instead bounce around the walls of the container. This state is called molecular flow, and it is the governing behaviour of these systems. The molecular volume flow rate across a cross-section of a tube is defined as the pumping speed \( S = dV/dt \) in litres per second. The pumping speed at the inlet of the pump is defined as \( S_p \). The throughput of the system \( Q \) is defined as the electrical analog of the system. It is related to the pressure of the system \( P \),

\[
Q = P \cdot S = (P_1 - P_2) C
\]  (2.1)
Where $C$ is the conductance of the system. The same electrical analogs apply to the conductance (such as in series $1/C = 1/C_1 + \cdots$, or parallel $C = C_1 + \cdots$). Throughout the system the throughput $Q$ is constant, and thus the pumping speed throughout the system can be translated through various connections and tubes through,

$$\frac{1}{S} = \frac{1}{S_p} + \frac{1}{C}$$

(2.2)

The amount of outgassing in a system will define the necessary pumping speed given some configuration of the vacuum system. The vacuum systems under molecular flow can be condensed down to two simplified conduction equations [20],

$$C_{\text{Pipe}} = 12 \frac{D^3}{L} \text{ [litre per sec]}$$

(2.3)

$$C_{\text{Aperture}} = 3.7 \sqrt{\frac{T}{M}} A \text{ [litre per sec]}$$

(2.4)

Vacuum systems are designed by considering the amount of outgassing occurring at the surface of the vacuum chamber. Then Eq. 2.1 is typically rewritten as,

$$P = \frac{Q}{S_p} = \frac{q \cdot A}{S_p}$$

(2.5)

Where $q$ is the outgassing rate of the material inside the vacuum chamber. Care must be taken to only select materials with low outgassing, and to prevent the formation of virtual leaks from trapped water or oils. Typical values for metal surfaces range from $10^{-7} - 10^{-8}$ torr liters per second per cm$^2$, and elastomer surfaces are around $10^{-5}$ torr liters per second per cm$^2$. The outgassing from water can be greatly reduced by baking the system, however, this usually requires special provisions (components must be able to withstand the heat), and as such the MIEL system is operated unbaked.

The MIEL vacuum system can be condensed down to two pipes. One is the main chamber which houses the main X-Y stage and other connections and feed-thorough, and another is the flexible hose which connects the main chamber to the turbomolecular pump. The flexible hose effectively reduces the pumping rate according to Eq. 2.2.

### 2.1.4 Cryogenic Cooling and Temperature Stability

SiPM devices are used in a range of temperature conditions. The device performances often change with temperature, so to match these, the SiPMs are mounted to a temperature controlled stage. The stage consists of copper braided connections to a cold plate, which is cooled through a LN2 suction loop.
Figure 2.8: Two examples of pumping down the vacuum chamber. The blue curve shows the proper trend of the turbopump evacuating the chamber (yellow region), and then entering the region where the system is dominated by outgassing (blue). The pressure continues to slowly decrease as outgassing lessens. The orange curve shows an example where there is a leak, or the backing pressure in the foreline is too high, and the pressure begins to rise after the pump slows down at constant power.
Table 2.2: List of current available laser heads for use in MIEL. All laser heads listed here are diode based, and thus have after-pulsing at high laser powers. All laser heads are diode coupled.

<table>
<thead>
<tr>
<th>Wavelength [nm]</th>
<th>System</th>
</tr>
</thead>
<tbody>
<tr>
<td>405</td>
<td>Picoquant</td>
</tr>
<tr>
<td>444</td>
<td>Hammatstu PLP-10</td>
</tr>
<tr>
<td>643</td>
<td>Hammatstu PLP-10</td>
</tr>
<tr>
<td>773</td>
<td>Hammatstu PLP-10</td>
</tr>
<tr>
<td>843</td>
<td>Hammatstu PLP-10</td>
</tr>
<tr>
<td>1296</td>
<td>Hammatstu PLP-10</td>
</tr>
</tbody>
</table>

LN2 is suctioned from a dewar, through vacuum jacketed connections through a feed through, and then looped through a copper cooling block. To cool the system effectively the majority of the dewar is placed above the cold plate.

The interior components of the vacuum chamber require consistent cooling for roughly 6 hours to reach a steady state equilibrium. If an appropriate amount of time is not waited, then the spacial position of the stage is not stable and can result in both x-y shifts or focus drifts. The effects of these are discussed more in Sec. 4.2.

2.1.5 Stimulation Lasers

MIEL is equipped to receive any fiber coupled laser source through a ThorLabs elliptical off-axis coupler. A list of current laser heads and systems available to the MIEL setup is shown in Table 2.2. The laser heads are coupled to a fiber, which allows them to be attenuated with a digital attenuator before being injected into the MIEL setup.

The goal is to stimulate a single SPAD on a SiPM device. The dimensions of the SPADs typically range from 35 µm, up to 60 µm, so the goal is to contain the focused spot entirely within the active area of that SPAD. This section briefly discusses the theory of focusing a laser spot to a point. For an assessment of the confinement to a SPAD, see Sec. 4.4.1.

The beam waist has two possible widths depending on how clipped the Gaussian wavefront is. The theoretical minimum width of a Gaussian beam focused to a point depends on the focal length $f$, wavelength $\lambda$, and the initial width of the beam $w_i$. Most specifications sheets for microscope objectives do not list the focal length of the objective, and instead supply the numerical aperture (NA). These relate together though the diameter of the objective pupil, $D$, and refractive index $n$. Thus the minimum spot size can be written as,

$$w_0 = \lambda f / \pi w_i = \lambda n D / 2 \pi w_i NA$$  \hspace{1cm} (2.6)
However, if the beam is sufficiently clipped ($D < 2w_i$) by the objective’s pupil, then the resulting focused spot is diffraction limited, and results in a Airy disk. The distance from the maximum to the first zero is,

$$d = \frac{2.44\lambda f}{D} = \frac{1.22\lambda n}{\text{NA}}$$  \hspace{1cm} (2.7)

The intensity of the beam is spread out more in an Airy disk rather than a focused Gaussian beam.

Another factor which influences the beam diameter sizing is the so-called $M^2$ parameter. This provides a measure for how much the beam spreads out from an ideal Gaussian beam. The resulting focused beam width is proportional to the ideal width by,

$$w_{\text{real}} = M^2 w_{\text{ideal}}$$  \hspace{1cm} (2.8)

### 2.2 Emission and Spectroscopy Measurements

After the light emitted from the SPAD is collected by the objective and filtered, it is direct to a Princeton Instruments spectroscopy system. This system is composed of a HRS-300 Pro, which is both a 300mm imaging system and scanning monochromator, and a PyLoN 400BR eXelon cryogenic camera.

The HRS-300 is based on the principle of the diffraction grating. The grating is made from a repeating pattern of specified period or spacing, $d$. The physical features may be different, ranging from square patterns to triangle shapes, depending on the application, however in principle, a plane wave incident at an angle of $\theta_i$ is diffracted to an angle $\theta_m$ of order $m$ according to,

$$d (\sin \theta_i - \sin \theta_m) = m \lambda$$  \hspace{1cm} (2.9)

The consequence of this relation is that when diffracting a wide range of wavelengths simultaneously, some wavelengths will overlap onto the same output angle. For example, if both 400 nm and 800 nm light are present, the first order diffraction of the 800 nm light will be contaminated by the second order 400 nm light. To navigate around this, a set of filters are chosen for specified wavelength ranges to avoid contamination from higher order diffraction.

The IX-83 microscope, which the MIEL setup is based around, contains two filter cube rotary turrets. Each rotary turret can house up to six filter cubes. Filter cubes can hold filters in three possible positions: horizontal, vertical, and diagonal.

The vertical filter is used for filtering out the incoming light, and is specified as the excitation filter. This can be used to filter out any secondary light from a light source. The horizontal filter is referred to as the emissions filter, and is typically used to remove stray or unfiltered excitation light. And the diagonal filter is typically a selective dichroic filter,
<table>
<thead>
<tr>
<th>Emission Wavelength Range</th>
<th>Choice of Filter</th>
<th>Stimulation Wavelength</th>
</tr>
</thead>
<tbody>
<tr>
<td>550-1100 nm</td>
<td>550 High Pass</td>
<td>&lt;500nm (405nm, 444nm)</td>
</tr>
<tr>
<td>400-800 nm</td>
<td>800 Low Pass</td>
<td>&gt;800nm (643, 834nm)</td>
</tr>
</tbody>
</table>

Table 2.3: List of current possible measurable wavelength ranges using the MIEL setup.

which is chosen to reflect the excitation wavelengths, and transmit the emission spectrum. The choice of three filters is usually done in tandem, and thus are included together in a filter cube. A list of possible filter configurations currently available to MIEL are shown Table 2.3.
Chapter 3

SiPM Surface Modelling

To deduce the spectral composition of photons directly produced from the avalanche from measurements performed with a microscope, an assumption on the structure of a SPAD must be made. Such modelling is additionally complicated by a number of undisclosed design parameters of the SiPM under test. Examples include proprietary anti-reflective coatings, location of the p-n junction within each SPAD, and other topological structures. However, the optical structure of a SPAD on an SiPM can be deduced down to an SiO$_2$ layer adjacent to a bulk Silicon layer where the avalanche occurs, at a point located $d_p$ from this surface. This level of modelling is often sufficient for modelling the transmission from the source of photons to an external detector.

The goal of this work is to develop a model of the photons at the source and calculate secondary photon emission, which heavily depend on the medium the SiPM is operating in. Thus the theory herein is kept quite general until it is utilized in very specific ways to model real world behaviour.

3.1 Optical Modelling

This section briefly discusses the main aspects of modelling optical phenomena relevant to SiPMs.

3.1.1 Attenuation in Media

All materials have some associated optical properties which can be characterized by associating them with a refractive index. To model both the refractive properties and absorption properties, we can set each material to have a complex refractive index written as,

$$\hat{n} = n_R - in_I$$  \hspace{1cm} (3.1)

Where $n_R$ is the refractive index, and $n_I$ is the extinction coefficient.

The bulk behaviour of light is that it moves as a wave through a medium. Additionally, these calculations are simplified by considering the complex form of a plane wave prop-
agating in the y direction. The resulting solution will be reduced down to its real form by considering only the magnitude of the resulting wave. With this in mind, we write the complex form of the wave,

\[
\vec{E} = \vec{E}_0 e^{i(\omega t - ky)} = \vec{E}_0 e^{i(\omega t - \hat{n}_y/c)} \\
= \vec{E}_0 e^{-\omega n_1 y/c} e^{i \omega (t - n_R y/c)}
\]

(3.2)

(3.3)

Where \(\omega\) is the angular frequency, \(c\) is the speed of light, and \(E_0\) is the initial electric field component. Here the link between the wave’s properties and the complex refractive index is made. The first exponential takes the form of the attenuation, which in general is described by,

\[
I(y) = I_0 e^{-\alpha y}
\]

(3.4)

Where \(\alpha\) is an attenuation coefficient of some form with the units \(m^{-1}\), and \(I_0\) is the initial intensity. In the case of light attenuation,

\[
\alpha = 2\omega n_1/c = 4\pi \nu n_1/c = 4\pi n_1/\lambda
\]

(3.5)

Where \(\nu\) is the frequency of the light, and \(\lambda\) is the wavelength of the light. By convention, we assume that we are always talking about the vacuum wavelength, and not the relative wavelength after the wave has moved between media. The value of \(y = \delta = 1/\alpha\) is known as the skin-depth, \(\delta\), which provides some measure of how far the light can penetrate into a medium. The smaller the skin depth, the less that the light will be able to penetrate into that media. For the majority of the optical modelling, Silicon is the dominate absorber over a wide variety of wavelengths. A plot of absorption vs entry angle into Silicon vs wavelength is shown in Figure 3.1.

### 3.1.2 Two Layer Fresnel Reflections

The theory for these calculations is taken from Ref. [11]. The transmission through the Si-SiO\(_2\)-\(n_3\) interface common with VUV-SiPMs can be described using the multi-wave reflection theory. The resulting wave which travels across the interface is a super-position of an infinite number of waves which have undergone reflection and transmission within the SiO\(_2\) interface.
Figure 3.1: Probability that light will transmit through the Silicon from a plane 0.145 µm deep to another plane located at 0 µm. The $y$-axis shows the angle the light is making in reference to the first surface surface, and the $x$-axis shows the wavelength of light emitted. The longer wavelengths are much less likely to be absorbed, and have a high probability of transmission. Wavelengths below 400 nm are unlikely to transmit far into Silicon. The bigger the angle of the light, the longer the path length between the two planes.
Snell’s Law

When a wave undergoes a change in medium, its angle of propagation changes at the boundary between the two media. This is classically described using Snell’s Law.

\[ n_i \sin(\theta_i) = n_t \sin(\theta_t) \] (3.6)

The standard textbook form is conventionally only valid for real \( n_i \) and \( n_t \), which are the refractive indices of the initial and final media, respectively. When the refractive indices are sufficiently different, a choice of initial angle may be beyond the so-called critical angle \( \theta_c \). When \( \theta_i > \theta_c \), the incoming wave will only reflect off the boundary. This critical angle can be found by taking \( \theta_t = 90 \), so,

\[ \theta_c = \arcsin(n_t/n_i) \] (3.7)

Though Snell’s law is conventionally shown with only real parameters, it works for the complex case too. If we use the complex \( \sin(z) \) functions, with real \( n \), then our real part will always be bounded by \( \pi/2 \). In later calculations, this regime will often result in zero transmission.

Fresnel Reflection Equations

Energy flows in the direction of the Poynting vector, which is given by

\[ \vec{S} = c^2\epsilon_0 \vec{E} \times \vec{B} \] (3.8)

Where \( \epsilon_0 \) is the vacuum permittivity of free space, and electric field \( E \) and magnetic field \( B \). It is only natural that the Poynting vector points in the direction of the propagation of the light wave. Ultimately what observable is the flux density (irradiance, W/m\(^2\)) which is given by,

\[ I = \vec{S}_T = \frac{\epsilon_0 c^2}{2} E_0^2 \] (3.9)

This allows us to model the behaviour of light using plane waves, and then ultimately reduce it to an irradiance to find what is actually measurable.

When a light wave encounters a single boundary, it is split into three field components: the incident wave, the transmitted wave, and the reflected. Let \( \vec{E}_i \) be an monochromatic wave incident onto a boundary from medium with refractive index \( n_1 \) to index \( n_2 \). The reflected and transmitted waves are given by

\[ \vec{E}_r(\vec{r}, t) = \vec{E}_{0r} \cos(\vec{k}_r \cdot \vec{r} - \omega_r t + \epsilon_r) \] (3.10)
and,

\[ \vec{E}_t(\vec{r}, t) = \vec{E}_{0t} \cos(\vec{k}_t \cdot \vec{r} - \omega_t t + \epsilon_t) \]  

(3.11)

Where \( \epsilon_r \) and \( \epsilon_t \) are phase constants, and \( \vec{E}_0 \) is the initial wave intensity. The \( r \), \( t \), and \( i \) indexes denote the reflected, transmitted and initial versions of these coefficients. Due to the conservation of energy, we require a boundary condition such that the field components are conserved,

\[ \vec{E}_{0i} + \vec{E}_{0r} = \vec{E}_{0t} \]  

(3.12)

By using Eq. 3.9 we can define the reflection and transmission in terms of the ratio of the time averaged power flowing through a surface \( A \) which bounds the two mediums.

\[ R = \frac{I_r A \cos(\theta_r)}{I_i A \cos(\theta_i)} = \frac{I_r}{I_i} = \left( \frac{E_{0r}}{E_{0i}} \right)^2 = r^2 \]  

(3.13)

and,

\[ T = \frac{I_t \cos(\theta_t)}{I_i \cos(\theta_i)} = \frac{n_t \cos(\theta_t)}{n_i \cos(\theta_i)} \left( \frac{E_{0t}}{E_{0i}} \right)^2 = \frac{n_t \cos(\theta_t)}{n_i \cos(\theta_i)} t^2 \]  

(3.14)

Where,

\[ r = \left( \frac{E_{0r}}{E_{0i}} \right)_{\perp \text{ or } \parallel}, \quad t = \left( \frac{E_{0t}}{E_{0i}} \right)_{\perp \text{ or } \parallel} \]  

(3.15)

The terms \( r \) and \( t \) are the so-called amplitude coefficient, and have different functional forms for s-polarized waves (slapping, perpendicular, \( \perp \)) and p-polarized waves (parallel, \( \parallel \)). These are explicitly given by Ref. [11],

\[ r_{\perp} = r_s = \frac{n_i \cos(\theta_i) - n_t \cos(\theta_t)}{n_i \cos(\theta_i) + n_t \cos(\theta_t)}, \quad r_{\parallel} = r_p = \frac{n_t \cos(\theta_t) - n_i \cos(\theta_i)}{n_i \cos(\theta_i) + n_t \cos(\theta_t)} \]  

(3.16)

\[ t_{\perp} = t_s = \frac{2n_i \cos(\theta_i)}{n_i \cos(\theta_i) + n_t \cos(\theta_t)}, \quad t_{\parallel} = t_p = \frac{2n_t \cos(\theta_t)}{n_i \cos(\theta_i) + n_t \cos(\theta_t)} \]  

(3.17)

It has been assumed that this is for dielectric material \((\mu_i = \mu_r = \mu_0)\). There are a couple of important relationships between the amplitude coefficient factors,

\[ t_{\perp} = -r_{\perp}, \quad \text{for all } \theta_i \]  

(3.18)

\[ t_{\parallel} = r_{\parallel}, \quad \text{for normal incidence} \]  

(3.19)

Notice that \( r_{\perp} \) can be negative, which indicates a phase shift with respect to the incident wave.
Figure 3.2: The ray travels through medium \( (n = n_1) \) until it encounters an interface \( (n = n_2) \). The ray then splits into an infinite number of other rays which are partially reflected within the middle medium. Rays that leave the interface only contribute to the field calculation. This Figure is summarized by Eq. 3.25.

For most calculations, we are working with the assumption that we have unpolarized light. To find the net transmission or reflection in this case, we take the average of the two possible polarizations,

\[
R = \frac{1}{2}(R_\perp + R_\parallel), \quad T = \frac{1}{2}(T_\perp + T_\parallel)
\]  

(3.20)

Two Layer Interfaces with Interference

We have described the behaviour of monochromatic waves at a single interface between a refractive index from \( n_i \) to \( n_t \). Next we wish to describe what happens when a light wave travels from a medium from \( n_1 \) to \( n_2 \) to \( n_3 \). It is expected that light will be reflected from the boundary from \( n_2 \) to \( n_3 \), and additionally reflected back from \( n_2 \) to \( n_1 \) (plus some transmission loss). This process can happen an infinite amount of times, and contributes to the overall transmission or reflection of the three medium system. Interference will be observed when these different light waves are recombined into one net transmitted wave. Figure 3.25 demonstrates this process.
We will define the transmission coefficient from medium $i$ to medium $j$ as $t_{ij}$ and similarly the reflection coefficient as $r_{ij}$. The functional form of the final reflection and transmission can be written as the sum of the field components,

$$\vec{E}_r = \vec{E}_{1r} + \vec{E}_{2r} + \vec{E}_{3r} + \ldots$$  \hspace{1cm} (3.21)

$$\vec{E}_t = \vec{E}_{1t} + \vec{E}_{2t} + \vec{E}_{3t} + \ldots$$  \hspace{1cm} (3.22)

We apply the phasor definition to a scalar version of the vectors rather than work with the vector form,

$$E = E_0 e^{i(\omega t + \delta_0)}$$  \hspace{1cm} (3.23)

Where $\delta_0$ is some phase parameter. When a ray travels through the medium $n_2$, the optical path length (OPL), with respect to the initial ray, changes by,

$$\delta = 4\pi n_2 d \cos(\theta_2)/\lambda_0$$  \hspace{1cm} (3.24)

Where $d$ is the thickness of the medium and $\theta_2$ is the angle inside the medium $n_2$, and $\lambda_0$ is the vacuum wavelength. The infinite series of phasor scalar amplitudes become,

$$E_t = E_0 t_{12} t_{23} e^{i\omega t} + E_0 t_{12} r_{23} t_{12} t_{23} e^{i(\omega t + \delta)} + E_0 t_{12} r_{23}^2 t_{12}^2 t_{23} e^{i(\omega t + 2\delta)} + \ldots$$  \hspace{1cm} (3.25)

$$= E_0 t_{12} t_{23} e^{i\omega t} \sum_{k=1}^{\infty} \left(r_{23} r_{12} e^{i\delta}\right)^{k-1}$$  \hspace{1cm} (3.26)

Ultimately the reflection field coefficients will be bounded by 1, and similarly, the complex form of $e^z$ is also bounded by one. Thus, since $|r_{23} r_{12} e^{i\delta}| < |r_{23}| |r_{12}| |e^{i\delta}| < 1$, the finite geometric sum formula applies safely,

$$s_n = a + ar + ar^2 + \cdots + ar^N = a \left(\frac{1 - r^n}{1 - r}\right)$$  \hspace{1cm} (3.28)

The infinite form of the geometric sum is taken under the limit when $n \rightarrow \infty$,

$$s_{\infty} = \sum_{k=0}^{\infty} ar^k = \sum_{k=1}^{\infty} ar^{k-1} = \frac{a}{1 - r}, \quad \text{for } |r| < 1$$  \hspace{1cm} (3.29)

Since the infinite sum is directly applicable to the infinite transmitted field, we apply it. This results in,
Figure 3.3: Plot of Eq.3.32, which is the transmission through an Si-SiO\textsubscript{2}-Air interface with $d_{\text{SiO}_2} = 1.34$ $\mu$m. The $y$-axis shows an angle of light with respect to the Si-SiO\textsubscript{2}-Air interface in the silicon. The $x$-axis is the vacuum wavelength of the monochromatic plane-wave. The oscillation present in the transmission is from the interference. The wavelength dependent critical angle can be seen between 400-1000 nm as the boundary from light to dark. Below 400 nm the light waves tend to form effervescent waves.

\[ E_t = E_0 e^{i\omega t} \frac{t_{12} t_{23}}{1 - r_{23} r_{12} e^{i\delta}} \]  

(3.30)

Since the light is unpolarized, both the parallel and perpendicular transmission and reflection field coefficients need to be taken. We then compute the transmission term,

\[ t_{\perp \text{ or } \parallel} = \left( \frac{E_0}{E_0} \right)_{\perp \text{ or } \parallel} = \frac{E_0 e^{i\omega t} t_{12} t_{23}}{1 - r_{23} r_{12} e^{i\delta}} = \frac{t_{12} t_{23}}{1 - r_{23} r_{12} e^{i\delta}}, \]

(3.31)

\[ T_{\perp \text{ or } \parallel} = \frac{n_3 \cos(\theta_3)}{n_1 \cos(\theta_1)} \left( \frac{t_{12} t_{23}}{1 - r_{23} r_{12} e^{i\delta}} \right)_{\perp \text{ or } \parallel} \]

(3.32)

An example of unpolarized transmission through an SiO\textsubscript{2} layer is shown in Figure 3.3.

### 3.1.3 Transmission from a Point Source

In a later section, we will be considering a point source of light located in the bulk material. If we want to write a function for the amount of light transmitted from that point source through some transmission function, we compute the indefinite integral,
\[
\int T(\lambda, \theta') \sin(\theta') d\theta' = F(\theta, \lambda)
\] (3.33)

And then the total amount of light entering a region is given by,

\[
A(\lambda) = \frac{F(\theta_2, \lambda) - F(\theta_1, \lambda)}{\int \sin(\theta) d\theta}
\] (3.34)

The denominator represents the total emission from the point source. This \(A(\lambda)\) factor behaves as a transmission, except over a set of angles from a point source.

### 3.1.4 Choice of Optical Properties

The optical properties utilized for this modelling come from a variety of sources. Since it is of great interest to understand SiPMs at the VUV wavelengths, the data sets chosen include these deep UV wavelengths. The Rochester Institute of Technology has an optical properties database for common semiconductor materials extending to 150 nm [33]. The RIT data set only includes wavelengths up to 800 nm, this is extended to 1100 nm by using the published data from Ref. [16], and Ref. [35]. Since it is of great interest to provide a model for the performance of SiPMs in LXe, using data obtained in either air or vacuum, the optical properties of LXe are also required and were obtained from Ref. [19].

### 3.2 Transmission into SiPM devices

The discussion of this section is largely for the verification of the theory outlined in the previous sections. Varying the angle of impinging light onto an SiPM device, and correlating it with the calculated transmission, showed that the above theory was applicable to modelling the behaviour of the Si-SiO\(_2\)-Air interface common in SiPMs.

After verification, the complete modelling of the optical features of the SiPM are then used to find the probability of photon absorption and subsequent avalanche. The modelling is then used to extrapolate the photon detection efficiency (PDE) measurement from a limited wavelength range (350-825 nm) to an extended range (100-1100 nm). However, the results contained within are an early effort, and do not match the published behaviour of the SiPM below 350 nm.

When modelling transmission into the SiPM device, the ray is reversed to that shown in Fig. 3.2. That is, the ray moves from \(n_1\) (air) to \(n_2\) (SiO\(_2\)) to \(n_3\) (Si). The modelling here also assumes that the photon is absorbed in the Silicon at the SiO\(_2\) interface.

### 3.2.1 The VERA setup

The Vacuum Emission Reflection Absorption (VERA) apparatus at TRIUMF is designed to collect SiPM response data over a broad range of wavelengths and various environmental operating temperatures. The experimental VERA team provided data of the photo-current
of an SiPM vs angle of the FBK-VUV-HD3 device, and the PDE at various voltages for the HPK-VUV4 device. The data in this work from VERA was collected by Harry Lewis and Nicholas Morrison.

### 3.2.2 Verifying with the FBK-VUV-HD3 Device

Angle vs current data was obtained using an FBK-VUV-HD3 device. The thickness of the SiO$_2$ layer has been measured using a commercial ellipsometer to be 1.34 $\mu$m. At small wavelengths ($\leq$450nm), the light current measured should be proportional to the transmission through the SiO$_2$ layer.

$$I(\lambda, \theta) = I_l(\lambda, \theta) - I_d(\lambda, \theta) = A \cdot T(\lambda, \theta)$$  \hspace{1cm} (3.35)

Where $I_l$ is the current through the SiPM with the lamp on, and $I_d$ is the current through the SiPM with the lamp off. The parameter $A$ is some constant of proportionality which takes into account intensity of the light and gain of the device. Optionally, if the gain of the device is known a-priori,

$$A = B \cdot G(V)$$  \hspace{1cm} (3.36)

And $B$ will depend only on the light flux. However, for this initial modelling, the gain of the device is not used. We are really only concerned with the following proportional relationship between the current measured and transmission,

$$I(\lambda, \theta) \propto T(\lambda, \theta)$$  \hspace{1cm} (3.37)

Which shows that a direct comparison can be performed. The current response at VUV wavelengths from 175 nm to 285 nm is shown in Figure 3.4, and visible wavelengths from 400 nm to 800 nm is shown in Figure 3.5.

Extra wavelength broadening has been applied to the transmission model to account for the range of wavelengths produced from the monochromator. The broadening factor depends on calibration provided by the manufacturer of the monochromator. This is accomplished by averaging equally over the expected wavelength resolution.

### 3.2.3 PDE Modelling with the HPK-VUV4 device

This section includes some additional theory for the absorption and avalanching of SiPMs from Ref. [14], to extend a previous Photon Detection Efficiency (PDE) measurement over a limited wavelength range to a much broader one. Classically, the PDE is written as,

$$\text{PDE}(\lambda, \theta, V_{ov}) = \text{FF} \cdot T(\lambda, \theta) \cdot \text{IPDE}$$  \hspace{1cm} (3.38)
Figure 3.4: The 1.34 µm SiO$_2$ transmission model applied to VUV wavelengths. A small broadening of 1.5nm has been applied due to the small slit size used. The model provides a good fit to the data for larger angles. Additional systematic effects may have influenced the data produced at small angles.
Figure 3.5: Fit optical model with SiO$_2$ thickness of 1.34 µm to VERA angle data for visible and near IR. Model assumes that the stage may not be perpendicular, or perfectly level, at $\theta = 0$. The resolution of monochromator was set to 9 nm, and so a broadening of 9 nm has been applied to the model.
Where FF is the fill factor of the device, $T(\lambda, \theta)$ is the transmission from the source of light to the Si, and IPDE is the internal PDE. The IPDE models the behaviour that the incoming photon is absorbed in the active region and causes an avalanche in the SPAD. This is a simplified model of PDE, and does not take into account the positional dependence on where the charge carrier is generated. In this section we will apply the position dependent model of PDE from Ref. [14], which is that probability of an electron or hole causing an avalanche can be considered as constant in their respective regions,

$$P_p(x) = \begin{cases} P_e, & \text{if } x \in [d^*_p, x_{pn}] \\ P_h, & \text{if } x \in [x_{pn}, d^*_w] \end{cases} \quad (3.39)$$

Where, $P_e$ is the probability of an electron causing an avalanche and $P_h$ is the probability of a hole causing an avalanche, and $x_{pn}$ be the center of the $p-n$ junction, and $d_w$ be the effective end of the depletion window and $d^*_p$ is the effective front. The space from the Si-SiO$_2$ interface to the effective start of the $p-n$ junction ($d^*_p$) is considered to be a so-called dead layer which is insensitive to incoming light. Effective regions are considered due to charge carriers being able to drift into the relevant regions, and this behaviour is nearly identical when looking at the SiPM response. Before the $p-n$ junction, the avalanches are entirely driven by electrons, effectively no holes contribute to causing the avalanche, and similarly, after the middle of the junction only holes contribute. When the photon is absorbed, it generates both an electron and a hole. However, wavelength of light largely decides where the electron-hole pair is generated. What follows is the calculation of the wavelength dependent probability of where the electron-hole pair is generated.

As the angle of the SiPM changes with respect to the incident light, the overall path-length changes within the silicon. If the light enters at an angle of $\theta$, then the path lengths change in the silicon according to,

$$x_{new}(\theta) = \frac{x_{old}}{\cos(\theta_{Si})}, \quad \sin(\theta_{Si}) = \frac{n_{air}}{n_{Si}} \sin(\theta)$$

Thus the probability of absorbing and causing an avalanche, given by Eq.3.39, is,

$$\text{IPDE}(\lambda, \theta) = \int_{d^*_p}^{d^*_W} \frac{1}{\mu} \exp\left(-\frac{x}{\mu}\right) \cdot P_p(x, V) dx = P_e \int_{d^*_p(\theta)}^{x_{pn}(\theta)} \frac{1}{\mu(\lambda)} e^{-x/\mu(\lambda)} dx + P_h \int_{x_{pn}(\theta)}^{d^*_W(\theta)} \frac{1}{\mu(\lambda)} e^{-x/\mu(\lambda)} dx $$

$$= P_e \left(e^{-x_{pn}(\theta)/\mu(\lambda)} - e^{-x_{pn}(\theta)/\mu(\lambda)}\right) + P_h \left(e^{-x_{pn}(\theta)/\mu(\lambda)} - e^{-d^*_W(\theta)/\mu(\lambda)}\right) \quad (3.42)$$
Figure 3.6: PDE of the HPK-VUV4 device measured by VERA. The results from the full data sets are shown.

Where $\mu(\lambda)$ is the attenuation length, and the equations utilize the angle dependent versions of Eq. 3.40.

The PDE data obtained using VERA over a set of operational over-voltages is shown in Figure 3.6. The PDE peaks at roughly 500 nm, and begins to collapse towards the shorter and longer wavelengths. The wavelength dependent behaviour for wavelengths shorter than 500 nm are governed by the transmission through the Si-SiO$_2$-Vacuum interface, and the electron avalanching probability. At longer wavelengths, the transmission through the Si-SiO$_2$-Vacuum interface is nearly constant, and thus the PDE is governed by the probability of absorption in the diode structure, and the hole avalanching probability.

Fitting Eq.3.42 is easily done after removing the effects of the Si-SiO$_2$-Vacuum interface, which is shown in Figure 3.7, where a subset of the over-voltages are given to show the systematic nature of the unknown, but constrained, SiO$_2$ thickness. This result, representing the probability of absorption and probability of avalanche after transmission, is known colloquially as the internal PDE. A nominal thickness of 125 nm was chosen for the remaining modelling, and the systematic bands are ignored. They are shown here to highlight how much the internal PDE changes over the 400-600 nm range, and performing the analysis over all regions leads to nearly no conclusions using the model here.

Fitting the plots with Eq. 3.42, results in the trends in Figure 3.8. The fit parameters for the electron and hole avalanching probabilities are shown in Figure 3.9 and the fitted $p – n$ junction parameters are shown in Figure 3.10. No assumption was made as to if any parameters are fixed over the change in over-voltage. Ideally, some constraint should
Figure 3.7: The bounds are defined by the range of possible thickness of the SiO2 layer of the HPK-VUV4 device. Dotted data points are for 125 nm SiO2 thickness. Only a subset of the total data from 1-8 $V_{oV}$ is shown. The dips at 400 nm are outliers.

Figure 3.8: Fitting Probabilities of absorption and avalanche with Eq. 3.42. This is also known as internal PDE as it does not contain any optical effects from outside the SPAD. Only a subset of the total data from 1-8 $V_{oV}$ is shown.
be placed on what the effective positions of the $p - n$ junction are, as the structure of the $p - n$ junction is not expected to change with voltage due to the constant single cell capacitance with over-voltage. However, the effective width of the junction may change due to the increase of avalanche probability with over-voltage. One interesting note is that the center position of the $p - n$ junction stays fixed at $0.81 \pm 0.1 \, \mu m$ which agrees with the assessment in Ref. [13]. There is not enough data below 400 nm to conclude the thickness of the dead layer, and so the model asserts that it is much smaller than the expected 5 nm. Using the model developed in this section to extrapolate the PDE performance over a wider wavelength range is shown in Figure 3.11.

3.3 Transmission out of SiPM devices

This section briefly discusses the optical modelling of the SiPM surface structure with regards to both the wavelength dependent transmission from the source of emission into an observing microscope objective with numerical aperture NA, and at all angles outside the SiPM for total emission from a device.

3.3.1 Transmission from Source to Microscope Objective

The majority of optical surface modelling is used to deduce the spectrum of light produced at the source of emission from a measurement of that emission. In this case, the source
Figure 3.10: Resulting quantities of $d_p^*$, $d_{pn}^*$, and $d_w^*$ by fitting Eq. 3.42 to the data shown in Figure 3.8. Note the uncertainties between $P_h$ and $d_w^*$ are highly correlated together. The results from the full data sets are shown.

Figure 3.11: The modelling performed in this section, and applied to extrapolate the PDE over the whole wavelength range of interest. Note that the $V_{oV}$ for the PDE provided in the HPK data-sheet was not provided. The impinging photon is never assumed to produce more than one electron, which may have an effect provided one of the generated charge carriers is outside the dead-layer and thus leads to an increase in the PDE.
of emission is assumed to be a point source located a distance $d_P$ within the bulk of the silicon as referenced from the Si-SiO$_2$ layer. Two fundamental assumptions are made for these calculations: the source of emission is isotropic and unpolarized.

MIEL has a number of microscope objectives with each of their numerical apertures,

$$\text{NA} = n \sin(\theta), \quad \theta_{\text{Si}} = \arcsin(\text{NA}/n) \quad (3.43)$$

The net transmission through the bulk silicon and surface layer are given by, $T_{\text{Si}}$, which is the transmission due to the attenuation in the Silicon, and $T_{\text{Si-SiO}_2-\text{Air}}$, which is the transmission due to the Si-SiO2 interface.

$$T(\lambda, \theta) = T_{\text{Si}}(\lambda, \theta) \cdot T_{\text{Si-SiO}_2-\text{Air}}(\lambda, \theta) \quad (3.44)$$

The amount of light, or probability of photon transport, we see is a ratio of the entire solid angle, by the solid angle seen by the objective,

$$A(\lambda) = \frac{\int_{0}^{2\pi} d\phi \int_{0}^{\theta_{\text{Si}}} T(\lambda, \theta) \sin(\theta) d\theta}{\int_{0}^{2\pi} d\phi \int_{0}^{\pi} \sin(\theta) d\theta} \quad (3.45)$$

Where $\phi$ is the rotational angle around the projection out of the SiO$_2$ surface. There does not expect to be any $\phi$ dependence on the emission, and thus is factored out in the final calculation. The assumption has been made that the source is isotropic (no angle dependence), and unpolarized.

A calculation using Eq. 3.45 was performed for both devices of interest in this study. The HPK-VUV4 transmission from source to microscope was calculated assuming a source depth of $d_p = 0.85 \, \mu m$, and $d_{\text{SiO}_2} = 0.1 \, \mu m$, and the FBK-VUV-HD3 transmission was calculated using $d_p = 0.145 \, \mu m$, and $d_{\text{SiO}_2} = 1.34 \, \mu m$. The systematic band on the FBK is small because of the confirmation of the SiO$_2$ thickness from ellipsometer measurements, and those measurements discussed in Sec 3.2.2. These transmissions are applied in Sec 4.6.2.

### 3.3.2 From Source to Total Photon Yield

After modelling the emission located at the source, a similar transmission calculation can be performed to identify the total number of photons emitted from the SiPM device. This quantity can be used to estimate the impact of external cross-talk on a detector system with a given photosensitive area. The calculations are performed for the medium which the SiPM will be operated in, to best match the expectations of performance of that device.

Similar to the section above, the calculation will be done in reference to some maximum angle present in the silicon, $\theta_{\text{Si}}$, from a point source located a depth $d_P$ into the silicon bulk. The maximum angle a ray can travel from the source in the Silicon is defined by the ray being parallel to the SiO$_2$ interface.
This calculation was performed in various media, as shown in Figure 3.14a and Figure 3.14b. These will be used in a later chapter to deduce the total photon emission of an SiPM in a media.

3.3.3 Summary

In this chapter we briefly outlined the theory of light in particular application to the optical surface structures found on SPADs and SIPMs. Care was taken to develop a general model applicable to most current SiPMs and potentially other future devices. The calculations used here are used in later sections to deduce further results of measurements performed using the MIEL setup, and extrapolate the impact of external cross-talk on a wider detector system.
Figure 3.12: Basic optical model of a SPAD. The light from the avalanche is produced at the surface located at $d_P$, and travels upwards. The photon may be absorbed in the green/gold-white gradient region, which dominates the transmission at smaller wavelengths and is governed by Eq. 3.4. The light grey region represents the SiO$_2$ optical interface and the transmission through this layer is governed by Eq. 3.32. The light grey oval represents the microscope objective.

Figure 3.13: Transmission functions for both devices from source of emission located in the silicon bulk to a 0.45NA objective located in a medium where $n = 1$. The systematic bands are derived from the uncertainty in the thickness of the SiO$_2$ layer.
Figure 3.14: Calculations for the transmission from source to anywhere outside the SiPM (Yield). The increased transmission in LXe and LAr are due to the better matched refractive indices with the SiO$_2$ layer.
Chapter 4

Data Analysis

4.1 Image Processing

MIEL is equipped with an Princeton Instruments PyLoN 400BR eXcelon cryogenic camera with an backside illuminated CCD sensor. The camera is specially designed for spectroscopic applications featuring a sensor with an aspect ratio of 1:3.35 and an array of 1340x400 20µm×20µm pixels. When the spectrograph is operating no zeroith-order, the 400 vertical pixels provide a spacial axis, and the 1340 pixels are mapped to some wavelength.

Let the response of a pixel be \( I[x, y] \), which is sometimes denoted as \( I[x, y, n] \) to show the pixel response of the \( n \)th frame. Multiple frames are taken over time to monitor the stability of the MIEL setup, which allows for monitoring X-Y stage drifts, Z-height/focus drifts, and cosmic rays. It is expected that the relative efficiency between pixels has been ignored due to its difficulty to measure and its small effect. As each pixel is read-out one at a time, the gain (\( \nu_{ADU} \)) is fixed for all pixels, this calibration parameter is instrument dependent and measured and reported by Princeton Instruments.

The read noise depends on the readout rate, with slower readout rates resulting in less noise. Emission measurements are 500s exposures, and the readout frequency of 50 kHz reads out the whole CCD sensor in \( \sim 10 \) s. The setting of 50 kHz is the lowest possible readout rate.

4.1.1 Cosmic-Ray Rejection

All long exposures from the CCD camera are susceptible to small tracks between pixels. These tracks come from cosmic rays ever present. A series of exposures from the MIEL CCD camera is shown in Figure 4.1, which show the random patterns these cosmic rays leave in each image. These cosmic rays are present on exposures taken of emission, and thus must be dealt with.

A set of \( N \) frames are reduced to a single frame by first identifying the cosmic-rays present per-pixel, then condensing the \( N \) pixels, ignoring pixels affected by cosmic-rays, to a single pixel.
The following cosmic-ray rejection method was chosen for its robustness. Cosmics-rays were first identified by taking the median ($\hat{I}[x, y]$), and then calculating the sample standard deviation:

$$\sigma_{N-1}^{2}[x, y] = \frac{1}{N-1} \sum_{n=0}^{N} (I[x, y, n] - \hat{I}[x, y])^2$$  \hspace{1cm} (4.1)

All pixel values $I[x_0, y_0, n]$ above $3\sigma$ above the median are rejected. Cosmic ray values are usually 1000 ADU above a real values. This process is shown in Figure 4.2a. If a pixel $I[x, y, n]$ has been identified as a cosmic, then all neighbouring pixels automatically become marked as cosmic too, and will be rejected. This process known as morphological dilation is shown in Figure 4.2b. This eliminates the effect of a high amount of charge generated in one pixel to affect the results of another.

After each pixel in a stack of frames is either identified as being affected by cosmic-rays or not, the following method is applied for computing the final pixel value in an image.

Take an average of the non-cosmic pixels $I[x, y]$. Then assign an error according to,

$$\alpha = \frac{\sigma_{N-1}}{\sqrt{N}}$$  \hspace{1cm} (4.2)

For short exposures (such as those used for efficiency calibration), this takes into account the change in incoming light flux (due to laser instability, lamp instability), or potential drifts in camera shutter speed.

If a background image ($I_{\text{dark}}[x, y]$) is present, then subtract it. Background subtraction is essential, as the amplifier has a pre-bias of $\sim 600$ ADU, and for longer exposures ($> 1$ hr) the leakage current becomes non-negligible.

An alternative method, but utilizing the same cosmic-rejection method, is to use the underlying distribution of pixels.

The read noise is, for most pixels, roughly Gaussian distributed, and can be measured from multiple background frames.

The light frame is a combination of Poisson counting statistics (photo-electrons or ADU per exposure?)

First apply cosmic-rejection and average the dark stack to find $I_{\text{dark}}[x, y]$, and $\sigma_{\text{dark}}[x, y]$. It is assumed that $I_{\text{dark}}[x, y]$ is just an bias offset applied in camera, and not leaked electrons.

$$I_{\text{light}}[x, y, n] = I[x, y, n] - I_{\text{dark}}[x, y]$$  \hspace{1cm} (4.3)

The summation of these pixels are shown in Figure 4.3. And the error,

$$\alpha[x, y, n] = \sqrt{I_{\text{light}}[x, y, n] + 2\sigma_{\text{dark}}[x, y]^2}$$  \hspace{1cm} (4.4)

Then find the average of the stack ($I_{\text{light}}[x, y]$), and then compute,
Figure 4.1: A sequence of exposures with background ionizing radiation shown in red. Tracks are randomly distributed over the whole frame, which indicate that these rays often do not overlap when comparing frames to each other in an exposure. Sources include muons, protons, and electrons generated from cosmic rays or other terrestrial background sources. Colour scale is emphasized to show the features due to ionizing radiation.

\[
\alpha[x, y] = \frac{1}{N} \sum_{n=0}^{N} \sqrt{I[x, y, n] - 600 + (\delta_{RN})^2} 
\]

(4.6)

Where the error from read noise, \(\delta_{RN}\), is assumed to be independent from the counting error. The read noise is provided by Princeton Instruments and is directly measured from our camera. Eq. 4.6 was the preferred statistical error for exposures with less than 25 individual frames, and thus was used for the majority of this work.

### 4.2 Data Diagnostics

A small set of data diagnostics were performed for each set of exposures. This is motivated by MIEL’s tendency to have stage or focus shifts if the interior of the vacuum chamber is not properly equilibrated by temperature. An example of a good set of frames is shown in...
Figure 4.2: The pictorial cosmic-ray rejection algorithm is shown in (a). A series of nominal valued blue pixels is contaminated by a cosmic-affect orange pixel. The mode and $4\sigma$ is calculated and found pixels above the required threshold, which become marked for rejection. Image (b) shows the technique for vetoing neighbour pixels which may be affected by the orange pixel.

Figure 4.3: A set of $N$ frames summed to one final image. The black pixels are marked as cosmic rays, and their neighbours will also be discarded.
4.3 Pulse Analysis

The output power of the laser for all MIEL measurements is set so that the SiPM will not fire on every laser pulse. To find the true number of avalanches during an exposure, additional pulse analysis on the output of the SiPM is required. This analysis characterizes the probability that the SiPM we fired at actually fired. Additional systematic effects are considered, such as distinguishing between stimulated pulses and dark pulses, or additional avalanches due to after-pulsing. A separate analysis was also performed with the setup to deduce the chance that another SPAD on the SiPM was fired instead of the one which the laser light was focused on. The following section discusses the characterizations performed on pulse level output of the SiPM for MIEL experiments.

4.3.1 Pulse Height Characterization

The electrical output of the SiPMs coincident with the laser signal was digitized simultaneously with an exposure of its emission. To avoid missing pulses from the SiPM, a pulse finder was not used and instead pulse analysis was performed over various regions. The first region \((R1)\) is located coincident with the laser trigger and a width of 200 ns. The goal of \(R1\) is to collect prompt pulses likely produced by the laser. An identical region \((R0)\) is located before the laser pulse with the goal of performing the same analysis, but where we expect only dark pulses. Lastly, another region \((R2)\) is located after the prompt region
Figure 4.5: Overview of the cosmic removal algorithm on a set of frames. Plotted in log scale.

(a) Raw sum of five individual frames to one frame.

(b) Cosmic-rays removed using the method of Sec. 4.1.1.

(c) Difference divided by the error in the final cosmic-removed image.
Figure 4.6: A waveform from the SiPM channel showing an SiPM pulse within the prompt region.

(R1) which seeks to characterize both dark noise rate, and after pulsing probability. Earlier systematic analysis utilized only the pre-trigger region (R0), which was replaced by using the post-trigger region (R2), which this section discusses. These regions are shown in Fig. 4.6

The analysis on regions of interest relies on distinguishing between different pulse heights. Due to the discrete nature of SiPMs, it is only needed to distinguish between the electrical baseline signal (0PE) and a single photo-electron (1PE). Charge or pulse height calibration is performed on the prompt region (R1). An example pulse height spectrum from R1 is shown in Figure 4.7. Initially a peak finder is used to approximate location of the 0PE and 1PE peak. Then, over a narrow fit region a Gaussian fit is performed and the parameters are extracted and used to calculate a linear formula for the location of the nPE peaks,

\[ f(n\text{PE}) = a \cdot n + b \]  

(4.7)
Figure 4.7: Histogram of pulse heights within the prompt region (R1). The peaks have been fit over a narrow region using a Gaussian function to extract their centroids.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$W_p$</td>
<td>Prompt (R1) Window Width</td>
</tr>
<tr>
<td>$W_d$</td>
<td>Delayed (R2) Window Width</td>
</tr>
<tr>
<td>$N$</td>
<td>total number of events</td>
</tr>
<tr>
<td>$N_{po}$</td>
<td>number of events with zero prompt avalanches</td>
</tr>
<tr>
<td>$N_{p1}$</td>
<td>number of events with only one prompt avalanche</td>
</tr>
<tr>
<td>$N_{po,d0}$</td>
<td>number of events with no pulses in either window</td>
</tr>
<tr>
<td>$N_{p1,d0}$</td>
<td>number of events with one event in the prompt window and one in the delayed</td>
</tr>
</tbody>
</table>

Table 4.1: List of parameters extracted from Fig. 4.8 and Fig. 4.9 used in the calculation of Sec. 4.3.2.

This re-scales the axis from charge (or pulse height) in terms of the photo-electron peaks. Thus for counting various outcomes from the SiPM, we can define all 0PE SiPM pulses (baseline) as taking the sum from $n = 0$ to $n = 0.5$, ie, halfway between the 0PE and 1PE peak. This charge (or pulse height) calibration from the prompt region (R1) is assumed to hold on the post-trigger region.

### 4.3.2 Dark Noise Rate

Correlation between pulse height in $R1$ and $R2$ is a 2D histogram shown in Figure 4.8. The x-axis shows the pulse height found in $R1$ and the y-axis shows the pulse height in $R2$. Sums over regions in this histogram, shown in Tab. 4.1, will be used to calculate the dark noise rate and after pulsing probability.
Figure 4.8: 2D-histogram showing the correlation between the prompt region ($R_1$) and delayed ($R_2$). The red vertical lines indicate the regions where pulses may be classified as 0PE or 1PE. Location of the centre of these regions is highlighted.

(a) Sums for $N_{p_0}$ and $N_{p_1}$.

(b) Sums for $N_{p_0,d_0}$ and $N_{p_1,d_0}$.

Figure 4.9: Measurements for raw parameters outlined in Tab. 4.1. Region of interests summed over are shown in green and purple. The total number of events ($N$) are summed over the whole histogram.
The probability that there is a SiPM pulse in the prompt region is given by,

\[ P_{R1} = 1 - P^0_{R1} = 1 - \frac{N_{p0}}{N} \quad (4.8) \]

Where \( P^0_{R1} \) is the probability of observing no pulses. The probability that a pulse is observed in the ROI (\( P_{R1} \)) cannot be used directly as a dark noise pulse is indistinguishable from an SiPM pulse which may have been triggered from the laser. To distinguish these two, an additional few steps must be performed to find, and apply the dark noise rate. Assuming that the probability that a pulse is found in a particular region of interest is Poissonian with an average rate \( r \),

\[ P(k \text{ events in interval } t) = \frac{(rt)^k e^{-rt}}{k!} \quad (4.9) \]

The probability that a dark noise event is seen in the delayed window is,

\[ P(0; W_d) = e^{-rW_d} = \frac{N_{p0,d0}}{N_{p0}} \quad (4.10) \]

The choice that a pulse is not seen in the prompt window is deliberate. If it is asserted that there is no pulse in the prompt window, then it has been at least 4\( \mu s \) since the previous laser pulse. The goal of this is to prevent contamination of after pulsing in the calculation of dark noise rate, under the assumption that the probability of seeing an after pulse after 4\( \mu s \) is small. Rearranging Eq. 4.10 for the dark noise rate,

\[ r_{dcr} = -\ln \left( \frac{N_{p0,d0}}{N_{p0}} \right) / W_d \quad (4.11) \]

Then the probability that the pulse observed in the prompt region (\( R1 \)) is not due to a dark pulse and is in fact a real pulse (\( P_l \)) is given by,

\[ P^0_{R1} = P^0_l \cdot P^0_{dcr} \]

\[ \rightarrow \]

\[ P^0_l = \frac{P^0_{R1}}{P^0_{dcr}} = \frac{P^0_{R1}}{e^{-r_{dcr}W_p}} \]

Thus,

\[ P_l = 1 - \frac{N_{p0} e^{r_{dcr}W_p}}{N} \quad (4.12) \]
4.3.3 After pulsing

Additional avalanches in the fired SPAD may occur, especially at higher over-voltages. These can be accounted for considering the delayed region for when there was a pulse in the prompt region. Under this condition, the delayed region is a mix of dark noise pulses and delayed correlated avalanches due to the main SiPM pulse.

\[
P_{p_1,d_0}^0 = P_{dr}^0 P_{cda}
\]

\[
P_{cda}^0 = \frac{P_{p_1,d_0}^0}{P_{dr}^0} = \frac{N_{p_1,d_0} \cdot N_{p_0}}{N_{p_1} \cdot N_{p_0,d_0}}
\]

Which assuming that correlated delayed avalanches are Poissonian,

\[
n_{cda} = - \ln \left( \frac{N_{p_1,d_0} \cdot N_{p_0}}{N_{p_0,d_0} \cdot N_{p_1}} \right)
\] (4.13)

However, this analysis assumes that there is little time dependence on the after-pulsing rate, which is often not the case. For example, the HPK-VUV4 device in this study has pronounced after-pulsing within the time scale of the first pulse, of which this analysis is unable to draw conclusions from. Instead, values for the number of correlated avalanches within 1 µs as reported by at many temperatures in Ref. [14] for the HPK-VUV4 device, and at LXe temperatures in Ref. [15] for the FBK-VUV-HD3 device. The interpolation scheme for the HPK-VUV4 device is shown in Figure 4.10.

4.4 Pre-trigger Analysis

The analysis on the pre-trigger region \( R_0 \) is identical to that which is performed on the post-trigger prompt region \( R_1 \). The purpose of this region is to be an alternative to the analysis performed in section 4.3.2 in the case that the method provided results which had nonphysical errors. This analysis constructs the “background” in the \( R_1 \) region, that is, contamination from either dark noise or after pulsing from a previous pulse.

After performing the pulse height analysis described in Sec. 4.3.1, as the counting is likely done on partial pulses, the probability of observing zero is computed. Once again, the probability of zero are those with heights less than 0.5PE.

\[
P_{R_0} = \frac{N_{<0.5PE}}{N_{all}}
\]

And the true firing probability is,
Figure 4.10: Number of additional avalanches within 1 $\mu$s of a prompt pulse for the HPK-VUV4 device. The interpolation has been performed linearly within the data points, and outside the points has been performed with nearest neighbour. Data points are taken from Ref. [14].

$$P_l = 1 - \frac{P^0_{R1}}{P^0_{R0}}$$

### 4.4.1 Hitting the Central SPAD

In the most ideal case, the microscope system would perfectly focus light onto a single SPAD. This can be verified by measuring the probability that an avalanche is seen with the amount that the laser light is attenuated. A simple model can be deduced for calculating the hit probability $P_c$, that is, the probability that a photon produced by the laser actually hits the center SPAD.

Per pulse, the laser emits $N$ photons, and the attenuator attenuates by a factor of $\alpha$. The number of photons reaching a SPAD from the laser after attenuation is,

$$n = N \times 10^{-\alpha/10}$$

Using the a-priori probability of causing an avalanche $P_a$, the probability that we see a central avalanche is modelled by,

$$P_{at} = 1 - (1 - P_cP_a)^n$$

And the probability that the laser causes an avalanche in another SPAD instead is,
Table 4.2: Parameters extracted by fitting models Eq. 4.14 and Eq. 4.15 to data presented in Fig. 4.12. The results of the fit are also shown in Figure 4.12.

\[
P_{ao} = 1 - (1 - (1 - P_c)P_a)^n
\]

We use these two terms to define explicit equations of what is observable from the SiPM through pulse analysis, and specifically only inspect the 0PE and 1PE outcomes. The equation for the probability of seeing no SiPM pulse, and only one SiPM pulse are given by,

\[
P_0 = (1 - P_{ac})(1 - P_{ao})
\]

\[
P_1 = P_{ac}(1 - P_{ao})(1 - P_{xt}) + P_{ao}(1 - P_{ac})(1 - P_{xt})
\]

The impact on the choice of \(P_c\) is show in Figure 4.11. Measurements were performed on a HPK-VUV-HD3 device. The results of this are shown in Fig. 4.12. Assuming a probability of a SPAD avalanche given it was hit by a photon \(P_a = 0.5\), both data curves were fit with Eq. 4.14 and Eq. 4.15 simultaneously. The results of the fit are contained in Table 4.2.

4.5 Spectral Emission

To obtain useful spectroscopic information, a number of calibrations and corrections must be made. As previously discussed, the total number of avalanches in an exposure must be known to deduce the emission per avalanche. This section discusses the steps required to develop these measurements, and produce a final number of photons measured per avalanche per wavelength,

\[
n_{\gamma}(\lambda) = \frac{N_{\gamma}^{cam}(\lambda)}{\epsilon(\lambda) \cdot N_{av} \cdot P_c \cdot (1 + N_{cda})}
\]

Where the number of avalanches is related to the total exposure time \(T\), and the repetition rate of the laser \(R_R\),

\[
N_{av} = T \cdot R_R \cdot P_f
\]

The \(N_{\gamma}^{cam}(\lambda)\) is the raw photo electron counts from the camera, normalized over bin width, \(P_c\) is the probability of hitting the center SPAD discussed in Sec. 4.4.1, and \(N_{cda}\) is
Figure 4.11: Equations 4.14 and 4.15 with two different choices of $P_c$. The perfect SPAD is modelled with $P_c = 1$ and the imperfect with $P_c = 0.5$. Both are assuming a cross-talk probability $P_{xt} = 0.11$, and an avalanche probability of $P_a = 0.5$. 
Figure 4.12: Probability of the number of photo-electrons measured given some attenuation on the incoming laser light. The lines depict the models Eq. 4.14 and Eq. 4.15 which were fit simultaneously to extract the parameters outlined in Tab. 4.2. $P_R$ quantity shows the probability that a pulse was greater than 1PE, and is not considered in the analysis. Errorbars are smaller than the datapoint markers.

the number of avalanches which may be missed when doing pulse counting over only the prompt region. Due to the difficulty using the ROI method discussed in the previous section to deduce number of delayed avalanches associated with a stimulated avalanche, values from Refs. [15, 13] were used instead. This provides only one value of $N_{cda}$ for FBK-VUV-HD3 at LXe temperatures, and a range of values for HPK-VUV4 from $-40^\circ$C to $-110^\circ$C. The rest of the values were interpolated using nearest neighbour.

The $\epsilon(\lambda)$ term denotes the MIEL setup’s optical efficiency from the microscope objective to the CCD camera. It is the topic of discussion in the following sections.

### 4.5.1 Wavelength Calibration

Wavelength calibration produces a set of coefficients $B[n]$ to form a non-linear calibration curve which converts x-pixel number ($n_x$) to a wavelength value,

$$\lambda(n_x) = \sum_{n=0}^{N_x} B[n] \cdot \delta[n - n_x]$$  \hspace{1cm} (4.18)

This is performed automatically using Princeton Instruments Intellical line source and software. Care is taken to select a slit size to have sufficiently narrow emission peaks from the source for an accurate non-linear wavelength calibration.
4.5.2 Relative Efficiency Calibration

The next stage is to use a calibrated light source over a wide range of wavelengths. The goal is to find the basic shape of the spectroscopic response of the whole system relatively. Initially a Princeton Instruments LED light source was used, but proved to be unreliable to calibrate over the whole spectrum. In its place, an Ocean Optics HL-3 spectroscopic broadband source was utilized, with a systematic uncertainty around 3% for most calibration points. The shape of the spectra was also ideal, with increasing intensity nearing where the CCD begins to lose sensitivity. The calibration points in between were calibrated using a spline interpolator, which can be seen in Figure 4.13. A breakdown of the calculation used to deduce the relative efficiency is shown in Figure 4.14.

4.5.3 Absolute Efficiency Calibration

To mimic a SiPM sample, a 0.22NA single mode fiber with a 50 µm core was placed in the sample position. The other end of the fiber is connected to a diode laser head of the
Figure 4.14: Process of calculating the relative transmission of the system. The drop off of efficiency below 550 nm is due to the emission filter. The decrease in efficiency past 1000 nm is dominated by the sensitivity of the cryogenic CCD camera.
Hammatsu PLP-10 controller. The power output of the fiber was measured for 1 hour before placement using a Thorlabs S105C fiber-coupled power meter. The total measurement time was necessary to account for the oscillatory power output, with a period of 10 min) of the Hammatsu PLP-10 laser diode. A set of (0.3s Exposure + 10s Readout)×300 exposures was taken to match the 1 hour of calibration performed. For both measurements, the repetition rate was the same.

The photon-electron rate is reported by the camera as,

\[ R_c^\gamma = \frac{\text{Total Photo-electron Counts}}{\text{Total Exposure Time}} \]  \hspace{1cm} (4.19)

Then the photon rate provided by the power meter is,

\[ R_{pm}^\gamma = \frac{\text{Power Measured}}{\text{Energy of a Single Photon}} \]  \hspace{1cm} (4.20)

The transmission is simply,

\[ T = \frac{R_c^\gamma}{R_{pm}^\gamma} \]  \hspace{1cm} (4.21)

To add support for this method, a set of transmissions from the components in the optical path were constructed, as shown in Figure 4.15. For locations of these various optical components, see Figure 2.2.

Inside the spectrograph there are three mirrors each with the same reflection transmission curve. This is taken into account in the entry “Spectrometer Reflection.” The spectrometer efficiency is taken only as a reference for these calibrations. Reported diffraction grating efficiencies are only reported for comparison between different diffraction gratings, and typically change with operating angle. Figure 4.16 shows a comparison of the resulting modelled curve, and the absolute efficiency calculated from two laser sources at 776 nm and 843 nm. The output wavelengths of the laser heads were verified using the wavelength calibration of the MIEL setup.

4.6 Spectroscopy Results

The previous sections discussed the various components of Eq. 4.16, which are now complete enough to perform spectroscopic measurements using the MIEL setup.

4.6.1 Measured Spectrum

A set of measurements were obtained for both the HPK-VUV4 device and the FBK-VUV-HD3 over a wide range of temperatures. Care was taken to match the temperatures of the two devices, but limitations in the temperature control scheme disallowed an exact match between the two devices. Both devices are designed to operate at LXe temperatures, so keen interest in this analysis was undertaken for the temperature points near 165°K (165°K for
Figure 4.15: Transmissions and efficiencies of individual optical components used to makeup the net model transmission presented in Figure 4.16.

HPK-VUV4 and 172°K for FBK-VUV-HD3). The measured spectrum into a microscope objective is shown in Figure 4.17 for HPK-VUV4, and Figure 4.18.

The oscillatory structure of the FBK-VUV-HD3 emission obscures some emission features, but both devices clearly have a downturn in emission above 1000 nm. And both devices show a steady increase in emission until 1000 nm. The principle component of emission is clearly from 700-1000 nm.

4.6.2 Source Spectrum

To find the emission located at the source inside the silicon bulk, the calculations employed in Sec. 3.3, explicitly the transmission located in Figure 3.13. The resulting spectra are shown in Figure 4.19 for HPK-VUV4, and Figure 4.20.

Now a comparison can be made between the spectrum produced by the two devices. Both spectra have the same peak at 1000 nm, and a slow rise from zero near 400 nm. Both spectra exhibit a “kink” near 700 nm which may give some indication in the method of photon production changing over this region.
Figure 4.16: Final MIEL Transmission utilized in this work. See text for how each component was calculated. The model transmission is composed of the individual transmission curves collected from data sheets and correspondences. The blue band shows the systematic uncertainty of the transmission curve.
Figure 4.17: Emission from the HPK device into a 0.45 NA objective. Statistical errors are shown as error bars, and systematic errors are shown as shaded error bands. Image (f) shows the integral of these spectra with only the systematic error common to each measurement.
Figure 4.18: Emission from the FBK device into a 0.45 NA objective. Statistical errors are shown as error bars, and systematic errors are shown as shaded error bands. Image (f) shows the integral of these spectra with only the systematic error common to each measurement.
Figure 4.19: Emission from the FBK device located at the source. Calculated using the transmission from Figure 3.13 applied to the spectra in Figure 4.17. Statistical errors are shown as error bars, and systematic errors are shown as shaded error bands. Image (f) shows the integral of these spectra with only the systematic error common to each measurement.
Figure 4.20: Emission from the FBK device located at the source. Calculated using the transmission from Figure 3.13 applied to the spectra in Figure 4.18. Statistical errors are shown as error-bars, and systematic errors are shown as shaded error bands. Image (f) shows the integral of these spectra with systematic errors.
Figure 4.21: Plots (a) and (b) show the spectra of the photons of the total yield from each device near $V_{oV} = 4 \text{ V}$. See Sec.3.3.2 for the discussion on how these spectra were calculated from the source emissions in Figure 4.20, and Figure 4.19.

### 4.6.3 Absolute Yield from HPK-VUV4 and FBK-VUV-HD3

For the situation where the devices will be installed in a actual detector system, either in room temperature in air, or in LXe, the total spectral emission was calculated using the calculations from Sec. 3.3.2.

In both situations, the FBK-VUV-HD3 device has a higher yield than the HPK-VUV4, though they are on the same order of emission. It is expected that both devices would impact a larger detector system similarly due to their similar emission shape. A summary of the non-spectral characteristics of both devices at 4 $V_{oV}$ are shown in Tab. 4.3. The spectra shown here are used in Figure 5.3 to calculate the actual impact on a toy detector system.

### 4.7 Preliminary Work

The final section in this chapter discusses work which is relevant, but is partially incomplete.

#### 4.7.1 Emission From PDC

Additional data was collected by MIEL of emission from the photon to digital converter (PDC). This device has the advantage of being actively quenched to suppressed any correlated avalanches, and the option of biasing one SPAD is available. This allows for improved consistency over the two analog SPADs reported in the previous sections.
Table 4.3: Summary of per avalanche and per charge carrier emissions for the HPK-VUV4 and FBK-VUV-HD3 device. Values are interpolated at $V_oV = 4$ V. Values in air are reported at room temperature, and values for LXe performance are reported at temperatures of 165$^\circ$K for HPK-VUV4 and 172$^\circ$K for FBK-VUV-HD3. Capacitance values for each device was taken from Ref. [15], and each device showed a non-constant trend with over-voltage which may indicate issues with pulse counting at low over-voltages. For reference other measurements of emission with charge carrier are, Ref. [27]: (500–1117 nm) $1.2 \times 10^{-5} \gamma/e^-$, and Ref [23]: [0.5-4.5] mA (413-1087 nm) $2.9 \times 10^{-5} \gamma/e^-$. 

<table>
<thead>
<tr>
<th>Device</th>
<th>Source Photon (at 293$^\circ$K) per Avalanche</th>
<th>Photon Yield/Avalanche</th>
<th>Air</th>
<th>LXe</th>
</tr>
</thead>
<tbody>
<tr>
<td>HPK VUV4</td>
<td>37 $\pm$ 7 $(1.5 \pm 0.3) \times 10^{-5}$</td>
<td>0.6 $\pm$ 0.2</td>
<td>1.2 $\pm$ 0.4</td>
<td></td>
</tr>
<tr>
<td>FBK VUV-HD3</td>
<td>56 $\pm$ 7 $(2.4 \pm 0.3) \times 10^{-5}$</td>
<td>0.8 $\pm$ 0.2</td>
<td>1.8 $\pm$ 0.4</td>
<td></td>
</tr>
</tbody>
</table>

A small preliminary data set was recorded at two temperatures. The data obtained from this is contained in Figure 4.22. Note that the emission below 700 nm is constant over the 100$^\circ$K operating range, while the emission above this threshold is changing with temperature. This could be used to characterize the emission mechanisms outlined in Ref.[3]. To convert the spectrum into eV (per unit energy) the following formula is used,

$$I_v(\nu) = c/\nu^2 I(c/\lambda)$$

The spectrum in electron-volts (eV) is shown in Figure 4.23, where a the spectrum at the source is shown following transmission calculations similar to what has been done on the HPK-VUV4 and FBK-VUV-HD3 devices.

### 4.7.2 Emission Maps

Emission maps are obtained when the spectrometer is operated in zeroth order mode, and thus only acts as a mirror. This allows for the spacial emission from an SiPM device to be deduced given a long exposure with the camera. The laser beam is focused onto a single SPAD at the centre of the image, and a filter is engaged to filter out the reflected light from the laser. Performing such a process produces Figure 4.24. Since we are only interested in SPAD-to-SPAD behaviour, the emission map must be digitized.

Digitization is accomplished by overlaying a grid onto the emission map, which is checked visually for correctness. This is shown in Figure 4.25, and Figure 4.26 shows the summed version of the image, but normalized by the light emitted by the central SPAD.
Figure 4.22: Emission from the Photon to Digital Converter (PDC) device. Note that the normalization on the y-axis is only per-pulse due to the data’s preliminary nature. Systematic error-bands shown in previous spectral plots have been omitted.

Figure 4.23: Source spectrum of the PDC normalized per eV to better match the source characterization performed in Ref. [3].
Figure 4.24: Emission map of a FBK-VUV-HD3 device. The cross-pattern should be correlated with the internal cross-talk of the device.

Figure 4.25: The red lines show the boundary of where each SPAD should be located. To process the data, the total number of photon counts is collected within each space. This gives rise to a “digitized” version of the emission map for analysis.
Figure 4.26: Total light emission from each individual SPAD, and normalized to the total number of counts within the central SPAD. This provides some measure of probability of triggering an avalanche in a neighbouring SPAD given an avalanche in the central.
Chapter 5

Conclusion

The work performed here has a number of implications both for the development of devices which rely on Geiger mode avalanches, such as SiPMs, as well as larger detector systems which utilize them. Secondary emission is clearly evident in SiPMs, and the amount of photons produced at the source ranges from 30-40 photons per avalanche at $V_{oV} = 4V$, which is a typical operating voltage for current generation blue sensitive SiPMs. The amount of emission per charge carrier remains on the magnitude of $1 \times 10^{-5}$ photons/e$^-$. On the SiPM level these cross-talk inducing photons can be mitigated by using optically opaque structures to separate individual SPADs on SiPMs. This however does not aid in mitigating cross-talk between different SiPMs in the same detector systems when the light escapes out the front of the SiPM. In this case external cross-talk will become the dominate processes over internal cross-talk when which SiPMs are designed to be operated at higher and higher over-voltages to improve detection efficiency and other performance parameters.

The effect of external cross-talk has only a small impact on detector systems which regularly observe large light signals, which can be calibrated out similar to how internal cross-talk is compensated for. However, this still leads to a measurable amount of degradation to a detector’s energy resolution. For detector systems which need to reliably detect small signals, or deduce physics results from only a few photons, such as dark matter detectors, the effect of external cross-talk is much bigger and single avalanches due to thermal induced avalanches could become confused with actual signals.

While this work largely focused on developing the method of measuring stimulated emission from SiPMs a few useful results and models were developed which allow for some results to be derived and directly compared with existing measurements. The first of which is to compare the magnitude of the effect of external cross-talk compared to the heavily characterized internal cross-talk parameter. The second is to make a comparison of external cross-talk probability between a theoretical toy LXe detector and LoLX using the same device.

The greatly simplified and theoretical toy detector is constructed by two assumptions, as shown in Figure 5.1: the transport probability of photons within the detector volume will
always be unity, and the entire surface of the detector volume is covered with SiPMs which are the same devices and have the same operating voltage. Due to this uniformity across the surface of the detector volume, light will be illuminating the target SiPM from any front facing angle. By combining some concepts developed in this work, the impact of external cross-talk can be estimated. The total light yield from SiPMs was developed in Sec. 4.6.3. Transmission from LXe to Silicon at any angle can be calculated through the use of of Eq. 3.32, but averaged over all possible angles measured from LXe, is shown in Figure 5.2 for the HPK-VUV4 device. The internal PDE values shown in Figure 3.8 give the detection probability if the cross-talk photon travels through the LXe-SiO$_2$-Si boundary. The result of the HPK-VUV4 transmission layer, internal PDE, and LXe emission is shown in Figure 5.3a. An interesting feature is that the most impactful range of emission is located in at $\sim$720 nm, and the effect of emission dies away further from this. The higher wavelength ranges is dominated by the PDE of the HPK-VUV4 device, and the lower wavelength ranges is due to the lack of emission. Integrating this spectra provides the number of additional photons that are detected per an avalanching SPAD, and provided a measure for the Poissonian parameter $\lambda$ introduced in Eq. 1.10. The total number of additional avalanches, as calculated by Eq 1.11 is shown in Figure 5.3b, where a comparison shows that the effect of external cross-talk for our toy detector is similar to that of internal cross-talk.

For a direct comparison of the external cross-talk using the toy detector with the LoLX experiment, Eq 1.7 can be used using the same HPK-VUV4 emission, optical surface trans-
Figure 5.2: Transmission calculation of light entering a HPK-VUV4 device from LXe. The transmission has been averaged over angles from 0 degrees from the normal to 90 degrees. This provides an effective transmission for light entering the SiPM from any possible angle.

mission, and internal PDE developed in the previous paragraph. Phase one LoLX also utilizes HPK-VUV4 devices, and has released preliminary data of the cross-talk probability presented in Ref [10]. The comparison between the LoLX data and the perfect toy detector is shown in Figure 5.4. The values obtained are similar, and provide an upper bound to those provided by LoLX, which is to be expected considering LoLX will have transport losses. In the future, the characterization of the LoLX detector system through Monte-Carlo simulation will provide a more accurate measurement of the impact of external cross-talk.

It is my hope that these measurements can be used to guide the continued development of new SiPM devices and mitigating internal cross-talk at the device level, and external cross-talk on the system level.
Figure 5.3: Effect of external cross-talk on a theoretical toy detector system using HPK-VUV4 devices. Image (a) shows the spectral light which is emitted from one SiPM and consequently detected by all other SiPMs in the detector system. Image (b) shows the total number of additional avalanches produced by external cross-talk (eCT) and a comparison is made with the additional prompt avalanches produced by internal cross-talk (iCT) from Ref. [14]. For the HPK-VUV4 device, external cross-talk has a similar effect as internal cross-talk.
Figure 5.4: Probability of causing at least one external cross-talk avalanche. The LoLX values are taken from Ref. [10], and the MIEL values are calculated using Eq. 1.7 assuming the transport probability $P_t = 1$. The MIEL values are an upper bound, which is expected.
Bibliography


Appendix A

Safety Analysis Reports

For the MIEL experiment to run, a safety analysis report was written to examine the risks involved with running the setup. It also serves as a training aid to using the setup safely. The safety manuals are available on request.
Appendix B

ANSYS Lumerical Application Examples

The following web-captures are of published application examples as a result of the MITACS 2022 Summer internship with ANSYS.

B.1 Modelling SiPM emission from a SPAD

This was an alternative method to producing the transmission plots in Sec.3.


B.2 Modelling Cross-talk between SPADs

This article outlines an attempt to model the internal cross-talk between SPADs using the emission at the source per avalanche, and making a comparison between emission maps.