MYTHEN CdTe: a new generation state-of-the-art X-ray imaging detector

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Abstract

MYTHEN is a single photon counting hybrid strip X-ray detector that has found application in X-ray powder diffraction (XRPD) experiments at synchrotrons worldwide. Originally designed to operate with hole collecting silicon sensors, MYTHEN is suited for detecting X-rays above 5 keV. However, many PD beamlines have been designed for energies above 50 keV where silicon sensors have an efficiency of only a few percent. In order to adapt MYTHEN to meet these energies, the absorption efficiency of the sensor must be substantially increased. Cadmium-telluride (CdTe) has an absorption efficiency approximately 30 times that of silicon at 50 keV, and is therefore a very promising replacement sensor material candidate. Furthermore, the large dynamic range of the pre-amplifier of MYTHEN and its capability to process charge carriers of either polarity has enabled the characterization of both electron and hole collecting CdTe sensors. A selection of Schottky and ohmic type CdTe MYTHEN test structures have undergone a series of characterization experiments including bias and settings optimization, energy calibration, count rate capability as well as stability tests of bias and radiation induced polarizations. The performance of those systems will be presented and discussed in this thesis.

Both, the radiation and bias induced polarization effects remained manageable. The MYTHEN system combined with CdTe sensors has proven to be reliable and stable despite high stress experiments. When biased over an extended period of time, the results of the studies have demonstrated that overdepletion of the sensors allowed the system to remain functional for a period of time 6 fold longer. During the high radiation studies, a count rate loss as well as a shift in threshold were observed, leading to the conclusion that individual charge carriers are been trapped. When applying a high bias as well as high flux, the detector system remained functional for 30 minutes. It was also demonstrated that a brief power cycle resumed normal performance after the system had shown symptoms of either polarization effect. Overall, the polarization effects observed on MYTHEN CdTe strip detector are temporary and show a slower impact than reported in the literature. Generally, a higher bias improved the stability of the detector.
Declaration

This is to certify that

1. this thesis comprises only my original work towards the PhD except where indicated in the Preface,

2. due acknowledgement has been made in the text to all other material used,

3. the thesis is less than 100,000 words in length, exclusive of tables, bibliographies and appendices.

Stefanie Romy Elbracht-Leong
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Introduction

In 1895, Wilhelm Röntgen discovered X-rays and changed the world. This Nobel Prize winning discovery allows us today to look through and inside optically opaque objects and samples. Since then the range of applications for X-rays has extended as wide as medical imaging, security screening, crystallography and powder diffraction, to name a few examples.

In any X-ray imaging experiments, the X-rays must be collected by some form of detector system in order to retrieve the information obtained in the course of the experiment. Over the years, the progress in imaging sensors has tried to match that of X-ray sources. However, the introduction of third generation synchrotrons as X-ray sources has dramatically improved the photon flux brightness, as well as time structure and monochromaticity of the beam. Unfortunately, the detector technologies have struggled to follow this rapid improvement. Quite often the detector deficiencies are the limiting factor of the experiments undertaken. In order to fully exploit the properties of modern synchrotron radiation, stringent requirements emerge with respect to the imaging system dynamic range, as well as energy, spatial and temporal resolutions. In order to satisfy these requirements, detector technology had to move from a traditional film system to a single photon counting method. State-of-the-art hybrid single photon counting detectors have been developed over recent years in an attempt to fully utilize the capabilities of synchrotron radiation.

MYTHEN\textsuperscript{1} is a single photon counting strip detector designed for powder diffraction experiments. The sensor material of choice has been silicon as it is a mature technology and fully characterized. However, it has limitations with respect to quantum efficiency when increasing the energy range. Silicon has an efficiency above 50 % for a 320 $\mu m$ thick sensor in the energy range of 3 - 16 keV. Increasing the silicon sensor thickness up to 1 mm extends the 50 % efficiency limit to 23 keV. However, this modest improvement is accompanied by significant signal degradation due to the possibility for the signal to

\begin{footnote}
\textsuperscript{1}Microstrip sYstem for Time-rEsolved experimeNts
\end{footnote}
spread further through the increased thickness of the detecting medium. An alternative approach to extending quantum efficiency is to replace the semiconductor with a high Z material. Cadmium-telluride (CdTe) is a suitable candidate due to its high quantum efficiency for photons of energy up to 100 keV with a 500 \( \mu \)m thick sensor and room temperature operation.

Discussed in this thesis is a comprehensive research study performed in order to narrow the source-detector capability disparity by improving the existing MYTHEN detector system via the introduction of a new CdTe sensor. A description of the thesis, chapter by chapter, follows.

Chapter 1 introduces X-ray production methods including laboratory setups such as rotating anode and third generation synchrotrons. Detection methods of those X-rays will then be explained as well as a list of the requirements of an ideal detector. This chapter will conclude with a comparison of the X-ray detector technologies currently available.

Chapter 2 reviews a variety of the key semiconductor physics that is paramount in the use of semiconductor photon detectors. A theoretical explanation of an effect, called polarization, affecting CdTe sensors will also be presented in this section.

Chapter 3 introduces the characteristics and functions of the updated MYTHEN detector system with a detailed description of key components of the readout chip.

Chapter 4 presents the results of primary characterization of the CdTe MYTHEN system obtained through a series of experiments performed in a laboratory environment as well as at the Swiss Light Source (SLS) in Switzerland. These results include the impact of bias and appropriate detector settings, energy calibration and resolution as well as count rate and dead time studies.

Chapter 5 discusses the results of polarization experiments performed at the Material Science beamline of the Swiss Light Source. It explains the results obtained from the stability tests under extended bias for multiple biases, as well as in two different high irradiation environments. The performance of the system under a high count rate within the limitation of radiation induced polarization is discussed. The purpose of this experiment was to test the limits of the detector system under extreme conditions before polarization affects the detection efficiency of the system.
X-ray Imaging Concepts

The discovery of X-rays was made by a German physicist, Wilhelm Röntgen, on the 8th of November 1895. He produced and detected electromagnetic radiation in the wavelength range now known as Röntgen rays or X-rays. Röntgen’s first X-ray image is shown in Figure 1.1. This advance in science was considered an achievement and earned him a Nobel Prize in 1901. Today, X-rays are used for a variety of applications including medical imaging, high energy physics, material science and security screening.

In this chapter the production of X-rays via a rotating anode and state-of-the-art synchrotron will be described, followed by an explanation of X-ray detection methods. Finally, the requirements of an ideal detector and a comparison of current detector technologies will be discussed.

1.1. X-ray production

In the scope of the study performed in this thesis, two different types of X-rays sources have been used. For the primary characterization of the detector presented in Chap-
Chapter 1. X-ray Imaging Concepts

Figure 1.1. Wilhelm Röntgen’s first X-ray, of his wife’s hand, taken on 22nd December 1895 [1].

In later work, the detector characterizations requiring very high flux and/or monochromatic X-rays were performed at the Material Science [2] at the Swiss Light Source (SLS) [3].

1.1.1. X-ray tube

X-rays are a form of electromagnetic radiation similar to visible light, gamma rays, radio waves, and microwaves. X-rays can be produced by accelerating electrons through a potential difference and scattering them towards a target material, typically tungsten. As shown in Figure 1.2, a heated filament (the cathode), will emit electrons via thermionic emission. Those emitted electrons will be accelerated towards the tungsten target, the anode, due to the high voltage difference. X-rays are generated in the tungsten either via braking radiation, also known as bremsstrahlung, or characteristic radiation.

Consider the case of energetic electrons which are scattered by a tungsten target. Some of these may encounter the positive charge of the tungsten nucleus, be deflected from their original path and lose kinetic energy in the process. This loss in energy is emitted as a bremsstrahlung X-ray photon, which can range from almost zero up to the kinetic energy of the incoming electrons. In some cases, an incoming electron may also collide with an inner shell electron of an atom in the target anode, leaving a vacancy in its place. The vacancy created can be filled by an outer shell electron. The atom which is now ionized and in an excited state can de-excite to a lower state, emitting an X-ray of
1.1. X-ray production

A typical X-ray tube in which electrons are accelerated from the heated filament (the cathode) towards a tungsten target material (the anode), via a high potential difference. The X-rays are generated within the tungsten either via braking radiation or characteristic radiation [4].

Specific energy, called a characteristic X-ray. An undesirable by-product of the process is heat. An increased temperature of the tungsten target would strongly limit the time under which the table top X-ray system could be used before breaking down. As the entire assembly must remain in vacuum to allow the electrons to reach the metal target, the anode is rotated in order to dissipate the heat.

A typical spectrum resulting from X-ray generation using an X-ray tube is shown in Figure 1.3. The spectrum can be manipulated by changing the voltage and current settings of the tube, as well as by adding filters between the tube and the object to image to eliminate low energy photons.

![Diagram of X-ray tube](image)

Figure 1.2. A typical X-ray tube in which electrons are accelerated from the heated filament (the cathode) towards a tungsten target material (the anode), via a high potential difference. The X-rays are generated within the tungsten either via braking radiation or characteristic radiation [4].

![Graph of X-ray spectrum](image)

Figure 1.3. Spectrum resulting from X-ray generation via an X-ray tube. The body of the spectrum is due to bremsstrahlung X-ray photons with energies ranging from 16 keV to that of the incoming electrons. Characteristic X-ray peaks are also visible at 57.98 keV and 67.24 keV [4] [5].
1.1.2. Synchrotron Radiation

Experimental results presented later in this thesis such as energy calibration or polarization studies required a high flux, highly focused, or monochromatic X-rays. The photon flux achieved by an X-ray tube is limited by the electrical current flowing through the tube. Maintaining the flux while spatially focusing the beam is also difficult. As can be seen in the example in Figure 1.3 the photon flux is a spectrum effectively ranging from 16 keV up to the applied electrical potential, and therefore not monochromatic.

In order to achieve the specific requirements of high monochromatic flux, the photon source has to be generated by a synchrotron light source such as the example shown in Figure 1.4. The source selected was the Swiss Light Source (SLS) in Switzerland and more precisely the Material Science beamline (X04SA) [2].

At the SLS, the electrons originate from the electron gun where they are thermionically emitted, similarly to an X-ray tube. They are subsequently accelerated to an intermediate energy of 100 MeV via a 5.2 m long linear accelerator, also called a linac. Electrons are then transferred into a 270 m circumference booster ring where their energy is increased up to the final energy of 2.4 GeV. Finally, they are injected into the 288 m circumference “third generation” storage ring. A series of bending magnets separated by straight sections guide the electrons. When deflected through the magnetic field, electrons emit electromagnetic radiation tangentially to their path. Those photons are optimized, primarily through monochromatisation and focusing, to meet specific needs of various beamlines. X-rays produced at the Materials Science beamline are in the energy range 5-38 keV with a maximum flux of $2.5 \times 10^{13}$ photons/s/0.4A at 10 keV.
1.2. X-ray interaction with matter

Photons can be used in a variety of different applications such as determining the structure of crystals or proteins, high resolution microscopy, spectroscopic analysis of atoms or medical imaging. All of these applications require the photons to interact with matter in order for them to be detected.

Photons have zero mass, are electrically neutral, and travel at the speed of light. Therefore, they do not steadily lose their energy via the Coulomb interaction. Rather they penetrate some distance within matter before depositing their energy via interaction with electrons or nuclei. Three types of interaction are applicable for photons: photoelectric effect, Compton scattering and pair production.

Prior to detailing each photon interaction type, the interaction probability needs to be introduced. The interaction probability of a photon per unit distance travelled is described by the exponential attenuation law \[I = I_0 e^{-\mu_{\text{att}}x}\] (1.1), where \(I_0\) is the initial photon flux and \(I\) the exponentially attenuated beam after passing through a material of thickness \(x\) with a linear attenuation coefficient \(\mu_{\text{att}}\). The
attenuation coefficient is defined as:

\[
\mu_{\text{att}} = \frac{n_A}{\rho} \sigma_{\text{tot}} \quad [g^{-1}cm^2]
\]  

(1.2)

where \(n_A\) is the number of target atoms per unit volume, \(\rho\) the material density and \(\sigma_{\text{tot}}\) is the total cross section for an interaction by the photon, frequently given in units of barns/atom (barns/atom), where \(b = 10^{-24}cm^2\). [7]

If the absorber is a mixture of different materials, the attenuation coefficient is the sum of the weighted average of its constituents:

\[
\mu_{\text{att}} = \sum_i \omega_i \mu_{\text{att},i}
\]  

(1.3)

Each individual interaction process will contribute to the total attenuation coefficient for a given energy and material, so that

\[
\mu = \mu_{\text{pe}} + \mu_{\text{ce}} + \mu_{\text{pp}}
\]  

(1.4)

where \(\mu_{\text{pe}}\) is the photoelectric effect attenuation coefficient, \(\mu_{\text{ce}}\) is the compton effect attenuation coefficient and \(\mu_{\text{pp}}\) is the pair production attenuation coefficient.

### 1.2.1. Photoelectric effect

As can be seen in Figure [1.5] for high atomic number (Z) materials and incident photon of energy less than 0.1 MeV, the dominant interaction process is the photoelectric effect [9]. In this process, a photon’s energy is transferred to an electron bound to an atom, subsequently followed by the emission of an electron. The recoil momentum of the released electron is absorbed by the residual atom. The energy of the incident photon has to be greater than the energy required to break the bond in order to transfer kinetic energy to the released electron [8]:

\[
K_e = h\nu - E_b
\]  

(1.5)

where \(K_e\) is the kinetic energy of the released electron, \(h\nu\) the incident photon energy and \(E_b\) the bonding energy.

Momentum conservation dictates that an incident photon can not be totally absorbed by a free electron [9]. However, total absorption of a photon can take place if the
1.2. X-ray interaction with matter

![Graph](image)

**Figure 1.5.** Respective dominance region of photon interaction processes (photoelectric effect, compton effect and pair production) as a function of the atomic number Z [8].

An electron is bound to an atom. The momentum conservation role is then assumed by recoil of the entire residual atom from which the electron was removed [8,10].

The probability of photo-electric absorption is greater for inner-shell electrons [10]. When this occurs, a hole is created which may be filled by the transition of an outer-shell electron resulting in the emission of either a characteristic fluorescent X-ray (radiative component) or an Auger electron (non-radiative component). A diagram of the process is shown in Figure [1.6]

The ratio of radiative to non-radiative transition is determined by [12]:

\[
\frac{N_k}{1 - N_k} = (-6.4 + 3.4 \times Z - 0.000103 \times Z^3)^4 \times 10^{-8}
\]  

(1.6)

where \(N_k\) is the fluorescence yield and \(1 - N_k\) the Auger yield. Up to an atomic number \(Z \approx 30\), the Auger electrons dominate. Above this \(Z\), both processes have approximately equal probability of occurring.
Chapter 1. X-ray Imaging Concepts

Figure 1.6. Photoelectric effect: the incident photon energy is transferred to an electron bound to an atom, subsequently followed by the emission of an inner shell electron (a). An outer shell electron will fill the lower energy inner shell space (b). The excess energy can either be released via a single characteristic fluorescence X-ray or be absorbed by an outer shell electron, causing its ejection from the atom [11].

The ejected photo-electron is emitted at an angle to the incoming photon, where the inner-shell differential cross section per atom describes the angular distribution [13]:

$$\frac{d\tau k_B}{d\Omega} = 4\sqrt{2r_e^2} \frac{Z^5}{137^4} \left(\frac{mc^2}{h\nu}\right)^2 \frac{\sin^2 \theta \cos^2 \phi}{(1 - \beta \cos \theta)^4}$$

(1.7)

where $\theta$ is the angle between the velocity vectors of the incident photon and the emitted electron, $\beta$ is the velocity of the emitted electron and $\phi$ is the angle between the incoming photon polarization direction and the scattering plane.

At low energy, the photo-electron is emitted almost perpendicularly to the direction of the incident photon. However, due to strong scattering with the lattice in a semiconductor, the range of the photo-electron is severely limited. The preferential directional emission therefore has minimal impact on the charge distribution and detector resolution.
1.2. X-ray interaction with matter

1.2.2. Compton scattering

In the incident photon energy range from 0.1 MeV to 10 MeV, Compton scattering (also known as the Compton effect) becomes the dominant interaction process. The Compton effect describes an inelastic scattering of the photon with quasi-free electron. A diagram of the process is shown in Figure 1.7.

For non-relativistic energies such that $\hbar \nu \ll m_e c^2$, the classical theory of Thomson which treats X-rays as classical electromagnetic waves is valid. In the Thomson theory, atomic electrons are regarded as free and oscillate at a frequency which is the same as the incident X-ray. Thomson demonstrated that each electron should scatter a definite fraction of the incident energy flux [8] and that this fraction is independent of the X-ray wavelength. Inherent in this theory is that the scattered and incident radiation have the same frequency [9].

By integrating the differential cross section over the entire solid angle of interactions, the Thomson scattering cross section can be calculated resulting in:

$$\sigma_{Th} = \frac{8\pi}{3} r_e^2 \ [cm^2/\text{electron}] \quad (1.8)$$

where $r_e^2 = \frac{e^2}{m_e c^2}$ is the classical electron radius.

The Thomson theory is not valid in a relativistic regime where $\hbar \nu$ approaches $m_e c^2 = 0.51$ MeV. The incident photon then has a momentum $\hbar \nu / c$ that can no longer be neglected. As both energy and momentum must be conserved, the photon transfers

![Figure 1.7. Compton scattering describes an inelastic scattering of a photon with an electron at rest [14].](image-url)
Chapter 1. X-ray Imaging Concepts

part of its energy to the electron which is then scattered at an angle \( \theta \) relative to the original photon direction. Conservation of momentum in the direction of \( \frac{h\nu_o}{c} \) is expressed by [8]:

\[
\frac{h\nu_o}{c} = \frac{h\nu_o'}{c} \cos \theta + p \sin \phi
\]  

(1.9)

where \( p \) is the momentum carried by the electron after the collision.

Conservation of momentum normal to the direction of \( \frac{h\nu_o}{c} \) is expressed by [9]:

\[
0 = \frac{h\nu_o'}{c} \sin \theta - p \sin \phi
\]  

(1.10)

Using Equations (1.9) and (1.10), as well as conservation of energy, one can define the energy transferred to the electron as [9]:

\[
K_e = h\nu_o e \frac{1 - \cos \theta}{1 + e(1 - \cos \theta)}
\]  

(1.11)

and that of the scattered photon as:

\[
h\nu' = h\nu \frac{1}{1 + e(1 - \cos \theta)}
\]  

(1.12)

where \( e = \frac{h\nu_o}{m_0c^2} \).

1.2.3. Pair production

For energies above twice the rest mass energy of an electron \( (m_0c^2 = 0.51 \text{ MeV}) \), a new interaction window becomes available: pair production [8][10]. Pair production occurs only in the electric field of charged particles, typically the nuclear field, as shown in Figure 1.8.

During pair production, the energy of the photon creates an electron-positron pair with total energy equal to:

\[
h\nu_0 = (K_{e^-} + m_0c^2) + (K_{e^+} + m_0c^2)
\]  

(1.13)

where \( K_{e^-} \) and \( K_{e^+} \) are the electron and positron kinetic energy respectively. Synchrotron radiation and medical imaging applications have insufficient energy to induce pair production in the detector semiconductor. This process typically occurs
1.3. X-ray detection methods

Each X-ray application has an individual set of requirements for a performing detector, such as energy range, energy resolution, cost, readout time.

For medical imaging, detectors must operate in an energy domain ranging from 17 keV for mammography [15] up to 150 keV for Computed Tomography (CT) [16] and 511 keV for Positron Emission Tomography (PET). Patient dose minimization, particularly in the case of a three dimensional CT reconstruction, is of utmost importance. The resolution of the detector will determine the minimum size of discernible features and is therefore a key characteristic of the detector.

In material science, for example X-ray fluorescence spectroscopy, a sample is irradiated and the characteristic X-rays emitted by the material are measured. Each material has a specific set of characteristic X-rays, allowing elemental composition to be determined. For such studies energy resolution is the critical factor. In synchrotron experiments, both position and intensity of X-rays must be precisely determined at a high flux. X-ray detectors therefore require high quantum efficiency, large count-rate dynamic range, as well as excellent time resolution.

Figure 1.8. Pair production: the high-energy incoming photon with energy $h\nu$ transfers its energy during the collision with the nucleus. Then, it creates a pair of electron and positron and passes kinetic energy onto each particle.

in high energy particle physics and is therefore outside the scope of this thesis. For further information, the reader is referred to [8][10].
Chapter 1. X-ray Imaging Concepts

In the discussion which follows, the salient properties of an ideal detector will be presented together with an explanation of direct and indirect X-ray detection techniques. Finally, cutting edge X-ray detector technologies will be compared.

1.3.1. Requirements of an ideal detector

Each application has specific requirements which define the acceptable limits of detector performance. In this section the most relevant characteristics of an ideal detector, such as energy resolution, spatial resolution, dynamic range, quantum efficiency, detector quantum efficiency, temporal resolution, radiation hardness, noise and count rate dynamic range will be discussed.

- **Energy Resolution** represents the ability of a system to distinguish photons closely separated in energy, and is quantified by the Full Width Half Maximum (FWHM) of the energy distribution, where an ideal response approaches the Dirac δ-like distribution. In practice, the spectral resolution should be sufficient to resolve features in the spectra under investigation.

- **Spatial Resolution** is the area over which a signal spreads out after impact at a single point, and is measured by either Point Spread Function (PSF), for a pixeleted detector, or Line Spread Function (LSF), for a strip detector, and its FWHM. The PSF (LSF) is the response of the detector to an ideal point (line) source. A slowly degrading PSF (LSF) can induce the signal to be artificially propagated to its neighboring pixels or strips [17][18]. In an ideal detector, only pixels or strips directly illuminated contribute to the image.

- **Dynamic Range** is defined as the ratio of maximal signal to the minimal detector signal, and quantifies the number of discrete measurements available.

- **Quantum Efficiency** is a measurement of the ratio of photons impinging on the detector that will produce an electron-hole pair. It is the detected fraction of incident photons [19]. The thickness and the absorption coefficient of the detecting material primarily dictates the quantum efficiency of the detector. Each photon should ideally produce a measurable signal in the detector proportional to the energy of the incident photon.
Quantum efficiency is generally not accessible to measurement, as the absolute number of incident photons is often unknown. On the other hand detector quantum efficiency, which is discussed next, is more easily measured.

- **Detector Quantum Efficiency** (DQE) describes how the input signal-to-noise ratio (SNR, described below) of a detecting system is transferred to the output SNR [20], and is defined as:

\[
DQE = \frac{S_{\text{out}}^2/\sigma_{\text{out}}^2}{S_{\text{in}}^2/\sigma_{\text{in}}^2}
\]

where \( S_{\text{out}} \) and \( \sigma_{\text{out}} \) are the average output signal and average output noise respectively [19]. \( S_{\text{in}} \) and \( \sigma_{\text{in}} \) are the average input signal and average input noise. DQE depends on the photon energy, efficiency of photon absorption within the detector volume, and readout electronics. In an ideal detector the DQE is equal to one, as all of the information from the incident beam is extracted by the system.

- **Temporal Resolution** represents the ability of a system to distinguish photons closely separated in time. Third generation light sources emit X-rays pulses with time-scales of the order of several tenths of picoseconds, whereas temporal resolutions of the order of several milliseconds are often adequate for the real time imaging of biological systems [21].

- **Radiation Hardness** is the dose of radiation that an X-ray detector can sustain before its performance is compromised or ultimately the detector rendered inoperable. Radiation induced effects on a sensor can be classified as either bulk or surface defects. Bulk damage includes the displacement of atoms, leading to changes in the electrical properties of the sensor [22]. Surface damage includes changes in the covering dielectrics and interface region [23] and manifests as an increase in leakage current and charge trapping [22].

- **Noise** is an undesired random perturbation in a detected X-ray signal and may originate from a variety of mechanisms. Phononic and dark noise are the two types affecting X-ray sensors.

Phononic noise is present in all systems and is due to fluctuation in the number of X-ray absorbed per unit area of detector. It obeys Poisson statistics and is formulated as the Signal to Noise Ratio (SNR) [20]:

\[
SNR = \frac{\Delta N}{\sigma} = \frac{\Delta}{\sqrt{N}}
\]
where $N$ is the mean number of absorbed X-rays and $\sigma = \sqrt{N}$ is its standard deviation.

*Dark noise* is produced in detectors when operating voltages are applied irrespective of whether external radiation is present. In a semiconductor dark noise is thermally generated and can be suppressed by cooling. In integrating detectors (described in Section 1.3.3) dark noise is always present and requires offline processing.

- **Count-Rate Dynamic Range** quantifies the usable range of a detector into the high-count rate regime. In an integrating detector it is the maximum percentage that the detector signal deviates from proportionality with input signal photon and is effectively infinite. Counting detectors require time to process a signal. A subsequent photon arriving within this dead time is effectively lost, decreasing the ratio of counted versus non-detected incident photon.

### 1.3.2. Direct and indirect X-ray detection

Depending on the energy of the incident photon, two detection methods are available: direct and indirect detection. In the case of direct X-ray detectors the incident X-rays are converted within the sensor itself. Direct detection allows for single photon sensitivity, as well as linear response and high spatial and energy resolutions. Indirect detectors utilize an intermediate scintillation layer to convert the primary radiation into visible light, which is then converted into an electrical signal in the semiconductor detector [20]. This method improves detector sensitivity at energies above 20 keV, and is favorable with respect to, as example, patient dose in medical imaging. Spread of light in conversion layers lead to a reduction in achievable SNR, contrast, and spatial resolution. Loss of optical photons and escape of K-edge fluorescence can also reduce SNR, contrast and spatial resolution. Furthermore, the relatively high energy of ~ 20 eV required to generate a secondary photon limits the achievable energy resolution [20].

### 1.3.3. Integrating versus Photon Counting Detectors

There are two prevalent and distinct approaches used in X-ray detector systems: integrating and photon counting.
1.3. X-ray detection methods

In an integrating system all incoming charges liberated by impinging X-rays are integrated during a predefined exposure time. This method has, in principle, an unlimited count rate dynamic range. However, the group treatment of all signals includes leakage and dark current noise, decreasing signal-to-noise ratio, dynamic range and limiting dose reduction in the case of medical imaging as example. Furthermore, in the integrating method, photon signals are weighted depending on their energy. Photons of higher energy deposit more charge in the detector resulting in a higher signal. In attenuation studies, lower energy photons are more heavily attenuated during the interaction with the object or sample being imaged, therefore carrying more information. Weighting photons by their energy decreases image contrast and signal-to-noise ratio.

In a photon-counting system, the charge produced is collected by a charge sensitive pre-amplifier, amplified and then compared to a predefined threshold set in a comparator. If the signal exceeds the threshold, the value of a counter is incremented. Each incident photon with an energy higher than that of the threshold has the same weight of one. Thresholding eliminates leakage as well as fluorescent background noise thereby achieving a noise free readout, increasing the signal-to-noise ratio and allowing a theoretically unlimited dynamic range.

A visual comparison of both principles of operations is shown in Figure 1.9.

1.3.4. X-ray detector technologies

A selection of the three most commonly used up-to-date and state-of-the-art X-ray imaging methods will be explained here: flat panel imaging, Charge Coupled Devices (CCDs) and hybrid photon detectors (HPDs).

- **Flat panel imagers** or Active matrix flat panel imagers (AMFPI) comprise of thin layers of amorphous silicon (a-Si) deposited onto glass substrates, with two-dimensional arrays of either thin film transistor (TFT) or thin film diode (TFD) fabricated on the a-Si. Those transistors are used as switches to control the readout of a photo-sensitive layer. Flat-panel X-ray imaging can be achieved either directly or indirectly.

In indirect detection systems, X-ray photons impinge first on a metal plate, primarily interacting via Compton scattering, creating a shower of electrons and Compton X-rays, which is then subsequently passed through a phosphorescent screen (usually Gd2O2S:Tb or CsI:Tl) [25] producing visible light. The visible
Figure 1.9. Comparison between integrating and photon counting detectors. In an integrating detector all signal is summed during a pre-defined exposure time, while in photon counting detector each photon signal is compared to a threshold. If the signal height exceeds the threshold, the value of the counter is incremented \[24\].
1.3. X-ray detection methods

light is then converted to an electronic charge by an array of TFT photodiodes residing below an amorphous silicon substrate.

Direct detection can be achieved via two different methods, the first of which uses an almost identical construction to the indirect detector, except that the phosphorescent screen is removed and X-rays are detected directly by the intrinsic layer of the photodiode [25]. The second type of direct detector replaces the photodiodes with a photoconductive layer of amorphous selenium (a-Se). Under the influence of an electric field applied across the photo-conductor, the charge cloud created by the interacting X-rays drift towards the surfaces of the photo-conductor where it is readout to a series of charge amplifiers at the bottom of the columns by the TFTs.

- **CCDs** are integrating charge-coupled devices comprised of a relay of electro-optical elements selected depending on the detector properties required. When X-rays are impinging onto a CCD detector, they are at first interacting with the luminescent material, usually a phosphor screen or semiconductor, and then converted into more readily manipulated visible and infra-red wavelength range. The light generated is then focused via an optical element, fiber optics and/or lenses, onto the smaller CCD chip, which generates photo-charges that are accumulated in an array of potential wells [26]. A depletion zone is created in the chip by gate electrodes on top of an insulating oxide layer. Charge packets accumulated into the potential wells are read-out by shifting them down pixel columns by a clocking gate. At the end of each column an analog output shift register transports the charge packets to a pre-amplifier and then an analog to digital converter before the next row is selected and read-out.

A consequence of individual treatment of the pixels is that the pre-amplifier senses only the capacitance of the last pixel, enabling very low noise. However, this creates a serial bottleneck readout, thereby limiting the readout time required for low noise read-out. Further, the CCD is continuously sensitive to radiation during readout. Therefore CCD often necessitates the use of high speed mechanical shutters to shield the detector.

Depending on the ambient temperature, electronic noise and dark current are present in the material of the sensor and the readout chip. A CCD chip integrates all these components together with the original signal, thus degrading the noise performance of the system.
Hybrid pixel detectors (HPDs) consist of a sensor inter-connected to readout electronics, allowing for independent optimization of both the read-out and the sensor. This separation is highly advantageous as the ideal substrate for particle detection is markedly different to that of an Application Specific Integrated Circuit (ASIC). Different sensor materials can therefore be used with the same readout, resulting in great design flexibility.

Furthermore, thanks to progress made in complementary metal-oxide semiconductor (CMOS) technology, the components required for advanced signal processing, such as discrimination and counting, are now able to reside in each pixel. In contrast to the detection techniques discussed above, this allows discrete photons to be counted and digitally stored in each pixel cell.

In HPDs, the sensor is segmented using the same geometry as the read-out chip. Each single detector is connected separately to a readout cell. The connection is provided by a small indium bump, which also provides mechanical stability between the chip and sensor. Thus allowing for the use of the digitalization within each pixel cell and process the acquired data in real time.

A more detailed explanation of the single-photon-counting HPD used in this thesis will be given in Chapter 3.
Solid-state materials may be categorized into three distinct groups: insulators, semiconductors and conductors. Conductors require little or no energy to promote an electron from the outer-shell, also called valence electron, into a conduction electron, for example via thermal excitation. In contrast, insulators require a significant amount of energy to break a bound electron in the valence state and promote it to a conduction electron. Semiconductors, as their name implies, lie in between these two extremes. At room temperature, thermal energy will not provide sufficient energy to promote a bound electron. However, the charge generated by the interaction of a keV X-ray is sufficient to liberate a bound electron into the conduction band and it is this feature of semiconductors which is exploited in X-ray detection.

A general description of semiconductors and their relevant characteristics will be briefly described in this chapter. For information beyond the scope of the thesis presented here, the reader is referred to [27]–[29]. An overview of the main properties of silicon, cadmium-telluride and other common semiconductor can be found in Table 2.1.
2.1. Semiconductors

2.1.1. Crystal Structures

In semiconductors the atoms are arranged along a small unit cell and repeated to form a three dimensional crystal lattice. Most commonly used semiconductors have either a diamond or zinc-blend lattice structure and are composed of two inter-penetrating face-centered cubic sub-lattices \[27\], as seen in Figure 2.1. Both the diamond and zinc-blend lattice types have tetrahedral structures in which each atom is surrounded by four neighboring atoms belonging to the second inter-penetrating sub-lattice. Each atom shares its outer valence electrons with those neighbors forming a covalent bond, thereby closing the outer shell \[27\].

Silicon (Si), which is to date the most commonly used semiconductor crystal, comprises a diamond lattice, whereas cadmium-telluride (CdTe) is a semiconductor crystal with a zinc-blend lattice, where each tellurium atom is surrounded by four cadmium atoms.

| Table 2.1. Summary of semiconductors main characteristics \[27,28\]. |
|---------------------------------|--------|--------|--------|--------|
| **Semiconductor**              | **Si** | **Ge** | **GaAs** | **CdTe** |
| atomic number                  | 14     | 32     | 31/33   | 48/52   |
| density \([g/cm^3]\)           | 2.33   | 5.32   | 5.32    | 6.15    |
| crystal structure              | diamond| diamond| zincblende| zincblende|
| band-gap \([eV]\) @ 300K       | 1.12   | 0.66   | 1.42    | 1.56    |
| average energy per e/h pair @ 300K \([eV]\) | 3.61   | 2.96   | 4.26    | 4.43    |
| carrier mobility @ 300K \([cm/s]\) | 1500(e), 3900(e), 8500(e), 1050(e), | 450(h), 1900(h), 400(h), 100(h), |
| direct or indirect band-gap    | indirect| indirect| direct| direct |
| dielectric constant \(\epsilon\) | 11.9   | 16.0   | 13.1    | 10.2    |
2.1. Semiconductors

Figure 2.1. Semiconductors crystal structures: diamond lattice on the left and zinc-blend lattice on the right. Both lattices are comprised of face-centered cubic sub-lattices. In the diamond case all atoms of the tetrahedron are identical, whereas in the zinc-blend crystal each sub-lattice supports a different atom. [27]

2.1.2. Energy Bands

As the atoms are brought together to form a lattice, their discrete energy levels broaden to form bands. Figure 2.2 shows the broadening of levels in the example of silicon atoms.

At sufficient lattice spacing, the conduction and valence bands are separated by a so-called forbidden or energy band-gap. The energy band-gap, $E_g$, is equal to the difference between the bottom of the conduction and the top the valence band and corresponds to the energy required to free an electron [28].

Figure 2.2. Energy levels of Si atoms arranged in a diamond lattice as a function of lattice spacing. [27]
Chapter 2. Semiconductor physics

The magnitude of the energy band-gap and, therefore, the electron occupation of the conduction band is a feature which defines a solid-state material. Metals, also called conductors, have a conduction band which is partially filled or overlaps the valence band as shown in Figure 2.3 (c-d). The energy gap can be large enough so that thermal energy or an externally applied electric field are insufficient to promote an electron from the valence band to the conduction band. In this instance, the valence band is fully occupied and the conduction band is empty, resulting in an insulator, as shown in Figure 2.3 (a) [27].

In a low temperature environment, the valence electrons remain bound to the lattice and no charge is available for conduction. As the temperature is raised to room temperature, thermal vibrations of the lattice can break the covalent bonds and render electrons available for conduction by exciting them over the relatively small band-gap. In the process, a deficiency commonly conceptualized as hole is created [27, 28].

A shift in deficiency location moves in the opposite direction of the electron under the influence of an external electric field and is therefore assigned a positive charge. Once the covalent bond is broken, both the electron and the hole are free for conduction and contribute to the electric current. The electrons in the conduction band and the holes in the valence band are relatively free to move about in the crystal, and can essentially be considered as classical charges with an effective mass dependent on the properties of the semiconductors.

Presented in Figure 2.3 is a simplified model of the energy band diagram to explain the differences between different solid-states and to define the relevant characteristics [27]. In reality energy band diagrams are significantly more intricate [30], as can be seen in Figure 2.4.

Figure 2.3. Energy bands structure for (a) insulators, (b) semiconductors, (c) and (d) conductors [27].
2.1. Semiconductors

Also represented in the diagram is the energy-momentum relationship of the conduction and valence bands. If the maximum of the valence band and the minimum of the conduction band are aligned, i.e. have identical wave vectors, an electron only requires sufficient energy to cross the energy band-gap. These types of semiconductors are referred to as direct semiconductors. In the case of an indirect semiconductor, the maximum of the valence band and the minimum of the conduction band are not aligned. For the electron to be able to make a transition across the energy gap towards the conduction band, sufficient energy is required, as well as a simultaneous momentum transfer to the crystal lattice. As can be seen in Figure 2.4, silicon is an indirect semiconductor, whereas cadmium-telluride is a direct semiconductor.

2.1.3. Fano Factor

As both energy and momentum must be conserved during the ionization process, a significant amount of energy will be dissipated to the lattice in the form of phonons. Therefore, the energy required to promote an electron to the conduction band, and thus create an electron-hole pair, is larger than the band-gap energy.

![Figure 2.4. Energy band diagram (also called energy-momentum relationship) of CdTe (a) and Si (b) [30]. CdTe is a direct semiconductor as the maximum of the valence band and the minimum of the conduction band are aligned. For Si the valence band maximum and conduction band minimum are shifted from each other. A momentum transfer as well as energy transfer is required to promote an electron from the valence band to the conduction band.](image)
The actual ionization energy $E_i$ can be presented by the following empirical expression [29, 31]:

$$E_i \approx 2.8E_g + 0.6 \text{ eV} \quad (2.1)$$

where $E_g$ is the band-gap energy. Taking silicon as an example, with a band gap of 1.12 eV and ionization energy of 3.6 eV at room temperature, only 30 % of the energy is converted into a detectable signal [29].

As the ionization energy is not entirely dedicated to breaking covalent bonds but will also be used for phonon excitation, multiple modes are available for energy and momentum transfer, yielding a fluctuation in the number of electron-holes pair created [29].

The absorption of incident energy $E_0$ deposited onto a sensor can be described by the following expression [29]:

$$E_0 = (E_{ion} \times N_{ion}) + (E_{lat} \times N_{lat}) \quad (2.2)$$

where $E_{ion}$ and $E_{lat}$ corresponds to the band-gap and the average phonon energy. $N_{ion}$ and $N_{lat}$ are, respectively, the number of ionizations and lattice excitations. As many combinations exist to dissipate the right amount of energy, the absorption of incident energy can vary from one event to another. However, the variations will average out over a long period of time. The variances of the total energy allocated to both processes is therefore equal to:

$$E_{ion} \times \sigma_{ion} = E_{lat} \times \sigma_{lat} \quad (2.3)$$

Using Equations 2.2 and 2.3 one obtains

$$\sigma_i = \frac{E_{lat}}{E_{ion}} \sqrt{\frac{E_0}{E_{lat}} - \frac{E_{ion}}{E_{lat}} N_{ion}}. \quad (2.4)$$

Each ionization forms a charge pair that contributes to the signal. The total number of charge pairs $N_Q$ generated is given by the total deposited energy $E_0$ divided by the average deposition energy $E_i$ required to produce one charge pair [27, 29]:

$$N_{ion} = N_Q = \frac{E_0}{E_i}. \quad (2.5)$$
The variance in ionization process is therefore

\[ \sigma_{\text{ion}} = \sqrt{\frac{E_0}{E_i} \sqrt{\frac{E_{\text{lat}}}{E_{\text{ion}}}} \left( \frac{E_i}{E_{\text{ion}}} - 1 \right)} \]  

(2.6)

where the factor on the right hand side is commonly referred to as the Fano factor \( F \) \[27, 32\]. The variance in charge pairs contributing to the signal is expressed as \[29\]:

\[ \sigma_Q = \sqrt{F N_Q}. \]  

(2.7)

In the case of silicon, \( E_{\text{lat}} = 0.037 \text{ eV} \), \( E_{\text{ion}} = 1.1 \text{ eV} \) and \( E_i = 3.6 \text{ eV} \), which yields to a Fano factor of \( F = 0.08 \) \[29\], smaller than a statistical variance \( \sigma_Q \approx 0.3 \sqrt{N_Q} \).

### 2.1.4. Intrinsic and Extrinsic Semiconductors

The probability of an electron occupying a state of energy \( E \) is given by the Fermi-Dirac function \[27, 29\]:

\[ F_n(E) = \frac{1}{1 + e^{\frac{E - E_F}{kT}}} \]  

(2.8)

where \( k \) is the Boltzman constant and \( T \) the temperature of the semiconductor. \( E_F \) is the energy at which the occupation probability of a state is half, and is known as the Fermi Energy. The probability of a hole state being occupied is:

\[ F_p(E) = 1 - F_n(E). \]  

(2.9)

Intrinsic semiconductors will contain very few impurities compared with the number of thermally generated electron-holes pairs \[27\]. Therefore the Fermi level of intrinsic semiconductors is centered within the band-gap. The level of purity required to produce intrinsic semiconductors is hard to obtain. Extrinsic semiconductors have therefore been produced by intentionally altering some properties of the material by adding impurities, a process called doping.

One can either obtain an n-type doped semiconductor with excess electrons in the conduction band or a p-type semiconductor with excess holes in the valence band. The type of semiconductor is the result of the replacement of an atom in the lattice by an atom with either more or fewer covalent electrons, as shown in Figure 2.5 on silicon \[27\].
Introducing impurities produces in a shift of the Fermi level towards the conduction band in the case of an n-type doping and towards the valence band for p-type semiconductor. See Figure 2.6 for an illustration.

Any excess of electrons in the conduction band or holes in the valence band can be considered as free particles as they are only weakly bound to the lattice.

2.1.5. Carrier Transport

There are two possible mechanisms which lead to the production of a current in a semiconductor X-ray detector. These relate to the motion of either the electrons in the conduction band and the holes in the valence band: either via application of an external electric field producing a drift or as the result of an inhomogeneous distribution of the

Figure 2.5. Doping of a semiconductor: by replacing an atom from the lattice with one containing either more or fewer covalent electrons than the original atom, one obtains respectively an n-type (left) or p-type (right) semiconductor [27].

Figure 2.6. Doping of a semiconductor: the introduction of impurities shifts the Fermi level towards the conduction band in the case of an n-type doping (left) and towards the valence band for p-type semiconductor (right). In the case of an intrinsic semiconductor there are no impurities changing the properties of the energy bands (center) [27].
charge carriers inducing diffusion. In either case both charge carriers contribute to the current and therefore the detectable signal.

Drift

As discussed in the previous section, the excess charges in their respective bands can be considered as essentially free particles. To account for the influence of the lattice, one attributes an effective mass $m_e$ to electrons and $m_p$ to holes. In the absence of any external influence, the charge carriers are free to move in all three degrees of freedom in the semiconductor. The thermal motion of the electrons is therefore a succession of scattering of the lattice or impurities within the sensor. As the motion is random, the effective displacement over time averages to zero.

If an external electric field is applied to the semiconductor, each electron will experience a Lorentz force from the field and will be accelerated along the field in the opposite direction, thus resulting in a non-zero displacement and a non-zero drift velocity is added to the thermal motion \[27,28\]:

$$v_n = \frac{q\tau_e \xi}{m_e}$$  \hspace{1cm} (2.10)

where $\xi$ is the applied electric field and the multiplication factor applied is the so-called mobility $\mu$, which is proportional to the mean free time $\tau_e$ and the charge $q$. Mobility is one of the main characteristics affecting signal collection, describing how strongly the charge carriers are bound to the lattice and is closely related to the time required to collect charges in a semiconductor detector sensor.

Scattering changes the dependency of the mobility on the temperature of the semiconductor. In the case of lattice induced scattering, the thermal vibrations of the lattice atoms will increase with temperature, implying an increase in energy transfer between the charge carriers and the lattice, therefore a decrease in mobility \[28\]. On the other hand, at higher temperatures the charge carriers have increased kinetic energy and

<table>
<thead>
<tr>
<th>Characteristic</th>
<th>Electron $[cm^2/Vs]$</th>
<th>Hole $[cm^2/Vs]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mobility CdTe</td>
<td>1100</td>
<td>100</td>
</tr>
<tr>
<td>Mobility Si</td>
<td>1400</td>
<td>480</td>
</tr>
</tbody>
</table>
therefore will remain in the neighborhood of the impurities for a shorter amount of
time causing a less effective deflection of their path due to Coulomb interaction \[28\].

As a consequence of their larger effective mass, holes have a reduced mobility com-
pared to electrons as is summarized in Table 2.2 for each charge type.

**Diffusion**

When the concentration of charge carriers is not homogeneous throughout the semi-
conductor, electrons and holes will move from a high density region towards a low
density region generating a diffusion current \[28, 33\]:

\[
J_n = q D_n \frac{\partial n}{\partial x} \tag{2.11}
\]

where \( \frac{\partial n}{\partial x} \) is the electrons density change along the x direction and \( D_n \) is the diffusion
coefficient \[28, 33\]:

\[
D_n = \frac{kT}{q} \mu_n \tag{2.12}
\]

with the charge \( q \), the Boltzman constant \( k \), the temperature \( T \) and the mobility \( \mu_n \).

Equations 2.11 and 2.12 are for electrons, but the same relationships are valid for holes
as well by replacing the mobility term appropriately.

**2.1.6. Carrier Generation and Recombination**

In this section the generation of charge carriers via either thermal vibrations or electro-
magnetic radiation will be discussed, as well as the direct and indirect recombination
mechanisms resulting from the departure from equilibrium conditions.

**Generation**

For semiconductors with a small band-gap, thermal excitation may be sufficient to
allow electrons to be directly promoted to the conduction band \[33\]. This type of
semiconductor detector must be operated at sub-room temperatures. If the band-
gap is larger than the thermal lattice vibrations, electrons can still be excited to the
conduction band via an intermediate center within the band-gap created by impurities
or imperfections within the semiconductor. In either case thermal excitation can be
detrimental to the semiconductor as it adds noise to the collected signal.
2.1. Semiconductors

Another generation mechanism results from the absorption of a photon with sufficient energy to bridge the band-gap. In the case of the absorbed photon having the same energy as the band-gap, an electron will be promoted to one of the available states in the conduction band. In the case of the photon having an energy larger than the band-gap, the promoted electron will occupy a state within the conduction band and subsequently de-excite itself towards the edge by either emitting a photon or a phonon. It is possible that an incident photon with energy smaller than the band-gap could still create an electron-hole pair in the presence of an impurity center within the band-gap as shown in Figure 2.7 [33].

Recombination

If the thermal equilibrium condition is disturbed, it can be restored by either a direct or indirect recombination process. If excess charge carriers are introduced in a direct semiconductor, the dominant recombination process is a direct band-to-band recombination. In indirect semiconductors the dominant recombination process is recombination via a center within the energy band-gap [27,28], which act as stepping stones between the conduction and valence bands as shown in Figure 2.8. The capture
Chapter 2. Semiconductor physics

of a conduction electron by a single-energy-level defect is shown in Figure 2.8(a). If 
the electron is emitted back to the conduction band after some time, Figure 2.8(b), the 
recombination site is vacant and can capture a hole from the valence band as shown in 
Figure 2.8(c). Hole emission, shown in Figure 2.8(d), can be viewed as the promotion 
of an electron to the valence band. Defects in the proximity to a band edge can capture 
a charge and release it after some time, a process called trapping shown in Figure 2.8(e).

Figure 2.8. Indirect generation-recombination processes available with a single-
energy-level recombination site [27, 34]. Electron transitions are 
represented by arrows. (a) Capture of a conduction electron by a single-
energy-level defect. (b) The electron is emitted back to the conduction 
band after some time. (c) The vacant recombination site captures a 
hole from the valence band. (d) Hole emission is the promotion of an 
electron to the valence band. (e) Trapping by defects close to either 
band edge, where a charge is captured and released after some time.
2.2. Semiconductor structures

Bringing two materials in contact, be they two semiconductors or a semiconductor and a metal, alters the characteristics of an interaction between an X-ray and the conjugate material. In this section pn-junctions and metal-semiconductor contact will be described along with their respective properties.

2.2.1. Pn-junction

A pn-junction is formed by joining two extrinsic semiconductors of opposite doping yields. While at thermal equilibrium, the Fermi level of each separated semiconductor is close to the valence or conduction band in the case of a p-type or n-type semiconductor respectively. As the semiconductors are brought together, the valence and conduction bands will bend to ensure that the Fermi level is constant across the entire device. An energy band diagram representing the bending behavior can be seen in Figure 2.9 [27].

Once the pn-junction is formed, electrons from the p-side will diffuse into the n-side as they travel from a higher to a lower density region. Similarly the holes will diffuse from the n-side into the p-side of the junction. The diffusion will uncover the respective donor and acceptor atoms, leaving a positive charge in the n-region and a negative charge in the p-region, introducing a build-up potential $V_{bi}$ and thus an electric field which will counteract the diffusion. The magnitude of the build-in

![Energy band diagram of the p and n-type semiconductors separated (left) and brought together (right). The Fermi level needs to be constant across the entire device. The energy bands therefore bent around it, creating a build-in potential $V_{bi}$.](image)
potential is dependent on the position of the Fermi level within the energy bands:

\[ V_{bi} = E_{fn} - E_{fp} \]  

(2.13)

where \( E_{fn} \) and \( E_{fp} \) are the Fermi levels within the separated n and p-regions respectively. Therefore, the build-in potential is a function of the level of doping in each region [29]:

\[ V_{bi} = \frac{kT}{q} \ln \left( \frac{N_A N_D}{n_i^2} \right) \]  

(2.14)

where \( N_A \) and \( N_D \) are the doping level of the acceptor and donor and \( n_i^2 \) is the intrinsic carrier concentration.

All charge carriers are swept away from the boundary region due to the electric field induced by the build-in potential, creating a drift current opposite to the diffusion current. The total current for the holes is thus:

\[ J_p = J_{p,\text{drift}} + J_{p,\text{diffusion}} \]  

(2.15)

\[ = q \mu_p p \left( \frac{1}{q} \frac{dE_i}{dx} \right) - kT \mu_p \frac{dp}{dx} \]  

(2.16)

where \( p = n_i e^{(E_i - E_F)/kT} \). A similar relationship can be found for electrons by replacing the hole carrier mobility with the appropriate electron mobility. At thermal equilibrium, the drift and diffusion current of the charge carriers cancel each other out, leaving the region around the junction boundary free of mobile charge carriers. This region is referred to as the space-charge or depletion region. The width, \( d \), of the depletion region is related to the build-in potential [27, 29]:

\[ d = \frac{2\varepsilon \varepsilon_0 N_A + N_D}{q \cdot N_A N_D} V_{bi}. \]  

(2.17)

The depletion region is a volume free of mobile charge carriers comparable to a capacitor where the undepleted p and n regions can be thought of as the electrodes and the depleted region as the dielectric [29]:

\[ C = \varepsilon \frac{A}{d} \]  

(2.18)

where \( \varepsilon \) is the dielectric constant and \( A \) is the area of the capacitor.
Applying an external bias to the pn-junction will cause departure from thermal equilibrium conditions. As can be seen in Figure 2.10, two options are available: forward or reverse bias. In the forward bias case, the positive side of the potential is connected to the p-region of the junction. As a result, the potential barrier is reduced, thus increasing the flow of electrons and holes across the junction.

The width of the depletion region can be increased by applying a reverse bias, where the positive side of the voltage difference is connected to the n-region, as:

$$d = \sqrt{\frac{2\varepsilon \varepsilon_0 N_A + N_D}{q N_A N_D} (V_{bi} + V_{rb})}$$

(2.19)
where $V_{rb}$ is the applied reverse bias.

Increasing the reverse bias will also decrease the capacitance of the device, thus increasing the signal charge while simultaneously decreasing the electronic noise.

Full depletion of the junction occurs when the externally applied reverse bias is equal to or exceeds the depletion voltage, $V_{dep}$. The quantity $V_{dep}$ is related to the effective bulk doping concentration, $N_{eff}$, by:

$$V_{dep} = \frac{q}{2\varepsilon\varepsilon_0}|N_{eff}|t_{junc}^2$$

(2.20)

where $t_{junc}$ is the junction thickness and $N_{eff} = N_D - N_A$.

There is, however, an upper limit on the reverse bias. At an electric field larger than $10^5 \, Vcm^{-1}$, electrons acquire sufficient energy to interact with the lattice and generate secondary electron-hole pairs [29]. Thus leading to the liberation of electrons from the valence band to the conduction band and destructive multiplication avalanches, resulting in a breakdown of the pn-junction.

If the pn-junction is irradiated while under the influence of an external electric field, the electron-hole pairs generated in the depletion region will separate and move towards their respective electrode in order to contribute to the detected signal.

### 2.2.2. Metal-Semiconductor Contact

A metal-semiconductor contact can be described similarly to the pn-junction in the previous section. Metals differ from semiconductors by their partially filled conduction band, as explained in Section 2.1.2. The Fermi level is therefore within the conduction band. Figure 2.11 shows the energy bands for the metal and semiconductor, n-type as well as p-type, separated and subsequently brought together.

A variable referred to as work function, $\Phi$, is the energy required to promote an electron from the Fermi level to the vacuum level. The electron affinity, $\chi$, is the difference between the edge of the conduction band and the vacuum level, and is a characteristic intrinsic to semiconductors, independent of doping levels [27].

Once the metal and the semiconductor are brought together, as for the pn-junction, the Fermi level needs to be homogeneous across the full device. The semiconductor bands
2.2. Semiconductor structures

Figure 2.11. Band profile of metal and semiconductor disconnected, (a) for n-type and (c) for p-type, and at equilibrium, (b) for n-type and (d) for p-type [27, 29, 33].
will therefore bend in the vicinity of the boundary as seen in Figure 2.11. A potential difference \( V_{bi} = \Phi_m - \Phi_s \) will build across the junction.

In the diagram (d) of Figure 2.11 a barrier is visible at the boundary 29:

\[
e\Phi_b = e(\Phi_m - \chi)
\]  

(2.21)

which is the threshold which an electron in the metal has to overcome to reach the semiconductor. This threshold is commonly referred to as the Schottky Barrier 29. The height of the Schottky barrier will not be altered by the application of an external voltage. On the other hand, the voltage difference \( V_{bi} \), which is the barrier electrons in the semiconductor have to overcome to reach the metal, will depart from equilibrium under the influence of an external voltage as shown in Figure 2.12.

Schottky type contacts behave similarly to a diode. Schottky sensors only allow current to flow in one direction due to the height of the barrier, and will therefore be referred to as Schottky diodes.

In the case of very high doping in the semiconductor (\( > 10^{19} \text{cm}^{-3} \)), the barrier height is greatly reduced and becomes sufficiently small for electrons to tunnel through 28,29. A metal-semiconductor contact with negligible contact resistance compared to the bulk or series resistance of the semiconductor is called an ohmic contact 27. In contrast to a Schottky diode, an ohmic contact can detect either one of the charge carriers current.

Figure 2.12. Band profile of a metal and a semiconductor junction under forward bias (a) and reverse bias (b) 27,29.
2.3. Polarization

In wide-energy band-gap semiconductor sensors such as CdTe, two separate polarization effects have been reported in various studies over the past two decades: bias induced \[35-38\] and radiation induced polarizations \[39, 40\]. The underlying mechanism for both effects will be described in this section.

2.3.1. Bias induced Polarization

Bias induced polarization is characterized by a gradual shift of the gain as well as a degradation in the spectral resolution, and has been observed in Schottky diode sensors but not in Ohmic contact sensors \[35\]. The main difference between both sensor types is the material used to form the anode. For CdTe semiconductors the cathode is generally made of platinum (Pt). In order to keep the Ohmic contact sensor properties symmetric, Pt is also the material of choice for the anode. On the other hand, Indium (In) is generally the material chosen to form the anode electrode in Schottky diode sensors due to its large Schottky barrier, creating therefore a blocking contact the In-CdTe junction.

The time scale reported for bias induced polarization is of the order of minutes. As reported in the literature, resetting the bias allows full recovery of the detector capabilities, rendering the bias induced polarization a reversible effect \[36\].

The exact origin or cause of the polarization effect is still a current topic of debate. However, there are indications that the responsible mechanism is related to hole detrapping from deep acceptor levels inducing a space-charge build up towards the anode \[36\]. After the application of a bias, the electric field will increase at the In anode and decrease at the opposite Pt cathode over time. The shift in electric field has been measured via the Pockels effect in a previous study \[36\]. As shown in Figure 2.13 after 60 minutes under bias, the electric field at the cathode is negligible. Over time the depletion region width is reduced on the cathode side of the sensor, rendering an increasing percentage of the sensor insensitive to incoming radiation, thus losing detection efficiency.

To date, the bias induced polarization effect has been attributed to deep acceptor levels, such as Cd vacancies, naturally present in the semiconductor. As can be seen in Figure 2.14 the deep acceptor levels can cross the Fermi level once the bands are
Figure 2.13. Bias induced polarization: under the application of a bias the electric field at the In anode increases while it decreases at the Pt cathode over time [36].

Figure 2.14. Energy Band diagram of Schottky-type CdTe sensor showing deep acceptor levels responsible for the bias induced polarization at equilibrium condition (a) and under reverse bias (b) [37].
bent to form a contact with the In electrode. Some deep acceptor levels are, therefore, already ionized before the bias voltage is applied \[37\]. Once a reverse bias voltage is applied, the holes Fermi level becomes greater than the deep acceptor level, creating a negative space charge due to the accumulation of those deep acceptor levels at the Schottky contact.

It has also been reported that the bias induced polarization effect can be improved by either lowering the temperature or increasing the bias voltage. Increasing the reverse bias will increase the depletion width beyond the thickness of the sensor, up to overdepletion. The electric field will, therefore, require more time to decrease to negligible value at the cathode \[36\]. Stability can also be improved at lower temperatures due to the larger ionization time of the deep acceptor levels \[38\].

### 2.3.2. Radiation induced Polarization

Radiation induced polarization is characterized by a decrease in count rate over time when subject to high radiation flux, dependent on the sensor material and pixel or strip shape and size. The reported time scale for radiation induced polarization effect is of the order of seconds to minutes, thus occurring before bias induced polarization, and the magnitude of the effect is dependent on the level of exposure to radiation \[40\].

A possible explanation of the mechanism responsible for the radiation induced polarization effect is the formation of a space charge due to the trapping of the low mobility holes generated by the incoming photons. If the generation rate of the electron-hole pairs exceeds the charge removal rate by recombination and drift rate, polarization will occur \[39\]. There is, therefore, a critical flux. Assuming the detector is illuminated from the cathode side, the incoming photon will penetrate in its vicinity and the critical flux \(\Phi_{\text{crit}}\) can then be described as \[39\]:

\[
\frac{1}{A} \Phi_{\text{crit}} \sim \frac{\varepsilon_0 V^2}{q L (\lambda \beta)^2} \left( \frac{\mu_h \tau_h}{\tau_h + \tau_{\text{drap}}} \right)
\]

where \(A\) is the area of the detector, \(\varepsilon_0\) the dielectric constant, \(V\) the applied bias voltage, \(q\) the elementary charge, \(L\) the device thickness, \(\mu_h \tau_h\) the holes mobility-lifetime product, \(\tau_{\text{drap}}\) the residence time of holes in hole traps and \(\beta = 1 - e^{-L/\lambda}\). As radiation induced polarization is due to a space charge build up due to the trapping of the holes, the hole properties are the main parameter in affecting the critical flux \[39\].
Chapter 2. Semiconductor physics

As the critical flux has been reached, the charge trapping produces a transverse electric field, which deflects the remaining carriers from their usual path, as shown in Figure 2.15. A further increase in the flux will increase the strength of the transversal electric field ultimately creating a pinch point as shown in Figure 2.16. Once such an extreme level of polarization is reached, no more charges can reach the anode.

Radiation induced polarization has been reported to be partially counteracted using two methods: increasing the reverse bias and an increasing temperature. Increasing the reverse bias increases the mean free path of the electrons and holes, thus decreasing

![Figure 2.15](image1.png)

**Figure 2.15.** Behavior of the electric field within a CdTe sensor under high flux radiation condition. The space charge build up creates a transverse electric field which alters the trajectories of the remaining charges [39].

![Figure 2.16](image2.png)

**Figure 2.16.** Behavior of the electric field within a CdTe sensor under a very high flux radiation environment. The space charge is sufficient to create a transverse electric field which forces all charge particles to meet at a pinch point. No charge can be collected at the anode [39].
their probability of being trapped. Turning the bias voltage off would imply a total recovery in the case of bias induced polarization, but only a partial recovery in the case of radiation induced polarization. An increase in temperature results in a decrease in trapping time of the holes ($\tau_{dtrap} \sim \exp(-E/kT)$).
MYTHEN: a Hybrid Single Photon Counting Strip Detector

MYTHEN (Microstrip sYstem for Time-resolved experiments) is a hybrid single-photon-counting strip detector designed by the Paul Scherrer Institute (PSI) detector group in Villigen, Switzerland. It has been developed for powder diffraction experiments such as those conducted at third generation light sources, including the Swiss Light Source (SLS) and Diamond Light Source [41]. The system currently installed at the Material Science Beamline (X04SA) [2] is capable of spanning 120° of a diffraction pattern within sub-second timing bins. Overall, this MYTHEN system consists of 40,000 channels acquiring independently in parallel and is optimized for time-resolved and dose-critical measurements [42]. MYTHEN modules are used also in several other types of experiments including energy dispersive spectrometry [43] and medical imaging [44, 45]. The modular structure of the MYTHEN design allows for custom arrays to be built to increase coverage area.

In the original design, and for all MYTHEN systems in operation to date, the semiconductor used as the sensor element is silicon (Si). As mentioned in Section [1, 3] one of the benefits of hybrid detectors is the flexibility in design and interchangeability of the sensing materials. The first section in this chapter will focus on a new semiconductor
Chapter 3. MYTHEN: a Hybrid Single Photon Counting Strip Detector

material proposed as the sensor for the MYTHEN system: cadmium-telluride (CdTe). An explanation of the functions of the read-out chip and the acquisition system will follow in the next sections.

3.1. Characteristics of the CdTe sensor

A silicon sensor of 300 \( \mu m \) thickness has a probability of interaction or quantum efficiency of 70\% at 12 keV, as can be seen in Figure 3.1. Although the attenuation efficiency decreases rapidly to 6\% at 35 keV, detection is still feasible under specific conditions as shown in Reference [46]. Medical imaging uses an energy range of up to 150 keV, resulting in a maximum efficiency of 1\% or below. Consequently silicon is inappropriate as a sensor material for high energy imaging detectors.

The quantum efficiency for a photon of energy \( E = h\nu \) is given by [47]:

\[
QE = 1 - e^{(E/T)}
\] (3.1)

![Figure 3.1. Quantum efficiency of a 300 \( \mu m \) (blue) and 500 \( \mu m \) (green) silicon sensor, as well as a 300 \( \mu m \) (red) and 500 \( \mu m \) (black) cadmium-telluride sensor. Plot generated using data from [7].](image)
where \( \mu \) is the linear attenuation coefficient of the sensor material as described in Equation 1.2 and \( T \) is the thickness of the detector. Therefore quantum efficiency can be improved by either increasing the thickness or atomic number of the sensor. To substantially extend the energy range available for imaging, a sensor material with a higher atomic number is required. Cadmium-Telluride is a compound material with a high atomic number (\( Z_{\text{Cd}} = 48 \) and \( Z_{\text{Te}} = 52 \) respectively). As shown in Figure 3.1, the attenuation efficiency of 300 \( \mu \)m of CdTe remains above 50% up to 70 keV. For a thickness of 500 \( \mu \)m, the attenuation efficiency is maintained above 50% up to approximately 86 keV.

The CdTe sensors used for this study were manufactured by Acrorad Co. Ltd (Japan) \[48\]. They have been constructed as 64 channels, each 500 \( \mu \)m thick single sided strips at a pitch of 100 \( \mu \)m, with a total length of 6.8 mm. Each sensor was bonded onto a ceramic interposer via gold studs with an approximate diameter of 60 \( \mu \)m and then subsequently wire-bonded to the MYTHEN read-out board as shown in Figure 3.2.

**Figure 3.2.** (a) A module with one silicon sensor and three CdTe sensors of the same geometry as the one characterized. (b) Schematic of the CdTe sensor bonded via gold studs onto a ceramic interposer, which is wire-bonded to a MYTHEN read-out board, including the dimensions of a single strip.
Figure 3.3 shows two different types of CdTe sensors that have been characterized. The first sensor type characterized in this study was an Acrorad CdTe ohmic contact, in which both electrodes were made of platinum working as a resistor, allowing collection of both charge carriers.

The second structure type had a Schottky diode contact between the CdTe bulk and indium-titanium multilayer anode, and an ohmic contact formed by a platinum layer as the cathode. The indium-titanium layer was formed by vacuum evaporation, whereas the platinum contact was fabricated by electroless plating [48,49]. Because of the large Schottky barrier at the indium contact, the Schottky diode worked only by collecting holes. A sensor with an aluminium contact as the anode has also undergone characterization. Due to the Schottky barrier formed by the aluminium layer and the CdTe bulk, this sensor collected electrons. Table 3.1 summarizes the sensors used.

<table>
<thead>
<tr>
<th>Sensor reference</th>
<th>Sensor type</th>
<th>Charge collected</th>
</tr>
</thead>
<tbody>
<tr>
<td>TS01-S</td>
<td>schottky</td>
<td>holes</td>
</tr>
<tr>
<td>TS02-O</td>
<td>ohmic</td>
<td>holes and electrons</td>
</tr>
<tr>
<td>TS03-S</td>
<td>schottky</td>
<td>electrons</td>
</tr>
<tr>
<td>TS04-O</td>
<td>ohmic</td>
<td>holes and electrons</td>
</tr>
</tbody>
</table>
In all of the tests, the sensors were back illuminated, i.e. the radiation impinged the side opposite to the gold studs and ceramic interposer in Figure 3.2 to provide a uniform absorption efficiency [50].

3.2. Analogue, front-end electronics

When X-rays are incident on the detector, they are absorbed by the CdTe sensor. The charge generated is collected at the electrodes and read-out is accomplished by custom developed front-end electronics. A MYTHEN module consists of 10 chips with a total of 1280 channels wire-bonded to the sensor. Each channel of the Application Specific Integrated Circuit (ASIC) is independent and can therefore be operated in parallel.

In each channel the signal from the sensor is passed to a charge sensitive pre-amplifier AC coupled to two shaping stages followed by a comparator, a pulse generator and a 24-bit counter [51]. By optimizing the gains of the pre-amplifier and shapers, as well as the comparator threshold, with respect to low noise and high count rate, the analogue chain can be adjusted to accommodate a wide range of applications. A schematic of the front-end chain is shown in Figure 3.4. Key components are described below.

The Charge sensitive pre-amplifier is the first element of the analogue chain. A 30 keV photon will deposit approximately $\sim 1 \, fC$ signal charge in CdTe. This charge is received and integrated by the pre-amplifier, producing a signal with amplitude

![Figure 3.4. Sketch of the architecture of a channel of the MYTHEN front-end electronics [51].](image)
Chapter 3. *MYTHEN: a Hybrid Single Photon Counting Strip Detector*

proportional to the energy of the absorbed X-ray. Overall, the charge gain is determined by an adjustable feedback capacitor, which can be tailored to meet the requirements of each experiment. Across the pre-amplifier, the voltage gain is defined as

\[ A = \frac{\Delta V_{out}}{\Delta V_{in}} \]  

(3.2)

where \( \Delta V_{out} \) is the output voltage and \( \Delta V_{in} \) the input voltage. Across the feedback capacitor \( C_{fb} \), the voltage difference is therefore

\[ v_{fb} = (A + 1)v_{in} \]  

(3.3)

and the charge deposited on \( C_{fb} \)

\[ Q_{fb} = C_{fb} \times v_{fb} \]  

(3.4)

where \( Q_{fb} = Q_{in} \) assuming the input impedance is null. Effective input capacitance is therefore defined as

\[ C_{in} = \frac{Q_{in}}{v_{in}} = C_{fb}(A + 1). \]  

(3.5)

Thus, the charge gain is \([29]\)

\[ A_Q = \frac{\Delta V_{out}}{\Delta Q_{in}} = \frac{A \times v_{in}}{C_{in} \times v_{in}} = \frac{A}{C_{in}} = \frac{A}{A + 1 \times C_{fb}} \approx \frac{1}{C_{fb}} \quad (A \gg 1). \]  

(3.6)

The signal gain is inversely proportional to the feedback capacitor.

Careful design of the pre-amplifier is crucial as the signal-to-noise ratio is dependent on the total capacitance of the sensor and pre-amplifier input. Furthermore, any internal noise must be minimised as it will be amplified along with the signal.

Next in the signal processing chain are two pulse *shapers* each AC coupled to the preceding stage. Similarly to the pre-amplifier, the shapers are tunable to adjust to the requirements of each experiment. In semiconductor detector systems the primary function of the pulse shaper is to optimize the signal-to-noise ratio \([29]\) and to differentiate the step function generated by the previous stage. As the frequency spectra of noise and signal differ, the signal-to-noise ratio can be optimized by applying a filter upon the frequency response and increasing the bandwidth of the pulse. The upper frequency boundary defines the rise time and the lower frequency boundary sets the
3.2. Analogue, front-end electronics

pulse duration or shaping time. The short shaping time of the analog signal permits counting individual rates of up to 1 MHz/channel \[42\].

As experiments can involve very high photon fluxes, pulses that are temporally close will lead to pile-up of successive signals, and therefore a loss of counts \[52\]. Compromise between minimal noise and high count rate capability must be decided for each individual experiment by optimizing the pre-amplifier and shapers settings. A qualitative study investigating the optimal detector settings is presented in section 4.1.5.

The next stage of the process involves the conversion of the analog signal into a digital signal via a discriminator. By comparing the signal amplitude with a pre-defined threshold, the system is capable of performing energy discrimination, allowing for rejection of noise as well as low energy fluorescence photons.

This threshold can be set globally by all channels by altering \(V_{th}\). Additionally, as can be seen in Figure 3.4, each channel has six programmable bits. One bit disables the channel while another puts the analog signal to the analog output of the chip. The remaining four bits are for the programming of the DAC, allowing each channels discriminator level to be individually trimmed.

An important feature of the MYTHEN discriminator is that the threshold is bipolar and therefore allows for the collection of both holes and electrons.

The output of the discriminator is connected to a 24 bit counter. If the signal is greater than the comparator threshold, the counter is increased by one. The counter is realized as a 24 bit shift register with an exclusive-OR feedback. This type of counter is also referred to as pseudo-random counter and has been thoroughly described in \[53\]. The advantages of such a counter include simplicity and compactness. One minor disadvantage is the randomness of the pattern generated, requiring off line decoding of the counter by use of a lookup table.

Partial read-out of the counter has been implemented to reduce the read-out and dead times. A digital control logic allows the readout of any number of bits per channel (normally 4, 8, 16 or 24 bits are chosen) \[51\].
Chapter 3. MYTHEN: a Hybrid Single Photon Counting Strip Detector

3.3. Data acquisition

The digital signals from each module are routed to a Field Programmable Gate Array (FPGA) which sends the control signals to the 10 custom designed 128-channel ASICs and returns the data to the acquisition system. The amplification and shaping parameters, as well as the status of the discriminator trim-bits and global thresholds, are controlled by the FPGA, as they are common to the 10 ASICs hosted on a module.

The FPGA is part of the MCS6 (MYTHEN control system 6), based on an embedded Linux system (ELS) \[50\] and able to control up to 6 modules. Both the FPGA and ELS are linked through the memory bus of the CPU. A fast data transfer is achieved by mapping the I/O registers of the FPGA to the ELS memory. The ELS runs at standard 100 MHz and communicates with the acquisition PC via a client server over a 100 Mbit Ethernet connection, with a maximum data transfer rate of 4 MByte/s. An external and dedicated PC controls the acquisition and read-out flow. All firmware has been designed and developed for real time data acquisition. A schematic of the architecture of the multiple modules MYTHEN data acquisition system is shown in Figure 3.5.

Note that as multiple prototype sensors were bonded to the same FPGA, a global trimming of the system was not used. The analyses presented in the following Chapters are, thus, performed on a strip-by-strip basis unless otherwise stated.
3.3. Data acquisition

Figure 3.5. Sketch of the architecture of the MYTHEN acquisition system [50].
This chapter reports on a series of experiments which were conducted to study the behavior, characterize and optimize the performance of several test detectors. Conventional current-voltage (IV) relationship analyses was used to investigate the bulk properties of the sensors. A controllable translation stage was used to raster scan the test sensors across a well defined beam of X-rays to study the bulk structure of the sensors. The inter-relationship between the bias voltage and settings on the detector response was also analysed. The results from these studies are presented together with energy calibrations, count rate response measurements, linearity studies and dead-time analysis.

4.1. Primary characterization

4.1.1. IV-Curves

Theoretical current-voltage (IV) responses are shown in Figure 4.1 for an ideal diode and resistor respectively. Any defects which may be present in the sensor will induce
a deviation from expected behavior. And so measurement of the current-voltage dependence analysis is a rudimentary check of the integrity of a semiconductor.

The device under test is placed in a circuit in which it can be biased selectively. An IV-curve can be then obtained by ramping the bias and measuring the current simultaneously. In the case of an ideal ohmic contact sensor, the current-voltage relationship is expected to behave like a resistor, linearly following \( I = V \phi R \). A Schottky type sensor IV-curve ideally qualitatively follows the shape of that of a pn-junction.

In the case of a diode, below the depletion voltage \( V_{dep} \), the depletion width follows Equation 2.19 and is thus proportional to \( \sqrt{V_{rb}} \), where \( V_{rb} \) is the bias applied. As the leakage current increases with the depletion volume, the IV response is also proportional to \( \sqrt{V_{rb}} \). As the depletion voltage is met and the depletion region spreads across the entire sensor width, the IV-curve reaches a plateau, which is the optimal region in which to operate the detector. As the electric field is further increased, valence electrons are released. The leakage current is thus increased, at first smoothly, and then rapidly turning into a breakdown as the sensor is irreversibly damaged.

\[ \text{Figure 4.1. Theoretical current-voltage responses for an ideal diode (red) and resistor (blue) \cite{33} \cite{54}.} \]
4.1. Primary characterization

The experimentally acquired IV responses of two Schottky and two ohmic sensors characterized in this study are shown in Figure 4.2. While the main plot is highlighting the plateau region of the IV-curve for the Schottky diodes and of the linear region for the ohmic contacts, the inset plots show the full voltage range over which the IV-curve for each sensor were performed. After each voltage increment and prior to each leakage current measurement, a waiting time of 60 seconds was applied. This relatively long settling time was selected to ensure the sensor current had truly settled. Each IV-curve was reproducible and repeated twice before and after undergoing primary characterization described below at the SLS. The IV-curves acquired for the sensors were all consistent with the theoretical model as well as the models described in Section 2.2.

The IV response of the ohmic contact sensors investigated were not perpetually linear, but rather showed a slowly increasing current towards a breakdown at either polarity of the bias. The breakdown is due to a small but non-negligible barrier at the metal-semiconductor contact interface creating space charge limited current [48, 55]. The IV response obtained also displayed a leakage current of almost two orders of magnitude greater than that of the Schottky sensors tested. A possible explanation of this leakage current magnitude difference is that the hole current in Schottky sensors was suppressed and the dark current was greatly reduced compared to that of the ohmic type sensor [48].

A series of measurement were undertaken to quantify the behavior of five different sensors:

1. Sensor TS01-S (Figure 4.2(a)) is a holes collecting sensor, with a forward bias breakdown starting at 900 V. At 400 V the leakage current is 3 nA and the lowest of all sensor studied.

2. Sensor TS02-O (Figure 4.2(b)), an ohmic type sensor, does not display a total symmetry between both bias polarities. The leakage current increases more rapidly with a negative bias. At 250 V the leakage current is 760 nA and -4.6 μA at -250 V.

3. Sensor TS03-S (Figure 4.2(c)), an electron collecting sensor, is a typical diode like behavior with a strong forward bias increase and, at a reverse bias of -700 V, the start of a breakdown. At a bias of -300 V the leakage current is about 30 nA.
Figure 4.2. IV-curves of the CdTe sensors characterized in this thesis.
4. Sensor **TS04-O** (Figure 4.2(d)) is an ohmic type contact displaying a symmetric IV-curve and has, at -150 V, a leakage current of about 200 nA.

Note that the abnormalities around -50 V in TS03-S are most probably due to the contact between the CdTe bulk and the Al anode as they are not present in the IV-curve for TS01-S which has an In anode instead.

### 4.1.2. Line Scan

A line scan measurement can be used as a detailed check of the sensor bulk for large defects and Cd or Te clusters created during the growth of the crystal. In order to perform this measurement, a 20 keV monochromatic beam at the Material Science beamline at the Swiss Light Source was collimated to 20 μm using precision slits in the vertical direction. The sensor was placed in the path of this beam and then scanned in 20 μm increments to produce a line scan. Examples of which are displayed in Figure 4.3 for sensors TS01-S and TS02-O and discussed below. The selected bias for sensors TS01-S and TS02-O were respectively 400 V and -250 V.

Referring to Figure 4.3, one can see the existence of two rows with reduced detecting efficiency visible at each vertical extremity of the sensors. These matched the positions of the gold studs used to connect the CdTe with the ceramic interposer. The ineffective regions under the gold studs did not affect the measurement as these could be corrected for using a flat field. Smaller efficiency loss regions, highlighted via red ellipses in Figure 4.3, are evident in most of the sensors. These regions are most probably Te inclusions within the Cd bulk. They are, however, sparse and affect a region of less than 60 μm in height. The apparent increase in efficiency towards the left side of the sensor TS01-S is attributed to inhomogeneity in the beam. This effect is only present in the line scan measurement for this sensor as each test structure was individually translated into the beam, thus using a different part of the beam profile.

On the top left of the line scan image obtained from sensor TS02-O, in Figure 4.3(b), a region of efficiency loss is visible, matching the position of a small portion of glue deposited on the sensor during the wire-bonding process. The glue has most probably diffused into the bulk of the sensor creating a defect. However, the impact of this region on the overall performance of the detector was limited, due to the position of this defect at the boundaries of the sensor which were not used as the main imaging region.
Figure 4.3. Linescan of the TS01-S (a) and TS02-O (b) sensors, performed with a 20 keV monochromatic beam vertically collimated to 20 μm via precision slits. Highlighted by red ellipses are potential Te inclusions. A small portion of glue was deposited onto the top left of sensor TS02-O during the wire-bonding process creating a defect as highlighted in orange. The non-normalized number of count is represented by the colour bar on the right hand side.
4.1.3. Detector response

In proper operation, a single-photon-counting detector is sensitive only to photons above a pre-defined energy threshold. Whilst providing an excellent measure of the count rate, the detector provides no specific information about the energy of the photon detected in this mode of operation. In order to extract more information on the energy spectrum of the photon beam, one can perform a threshold scan in which the comparator level is incrementally varied over a pre-defined range, allowing the study of detector energy dependance.

In Figure 4.4, the dash-dotted blue line represents a theoretical threshold scan of an ideal detector placed directly in the path of a beam of perfectly monochromatic X-rays. In this case the detector counts all of the incoming photons until the threshold energy, 20 keV in this example, is reached. When the threshold is raised above the photon energy, no counts are registered, resulting in an extremely sharp edge or step.

![Figure 4.4](image)

**Figure 4.4.** Expected counts for a threshold scan performed with monochromatic X-rays of 20 keV. The detector absorbs 10000 counts during the exposure time. The dashed dotted blue line represents an ideal detector with no electronic noise or charge sharing. The solid green line shows the effect of ENC = 2 keV but no charge sharing. The dashed magenta line represents the number of photons with their entire charge cloud collected by a single strip. Finally, the solid red line is a realistic detector with an ENC = 2 keV and charge sharing of 10% and the corresponding fit to determine the ENC in black.
In a more realistic case, a threshold produces the curve as shown in Figure 4.4 as the solid red line. This curve is commonly referred to as a Sigmoid or S-curve. S-curves provide vital information on the quantum efficiency of the detector and are a crucial tool in characterizing and optimizing the settings of the system for each experiment. The S-curve for a monochromatic beam is described by the following equation [56]:

\[
C = \text{Erf}\left(\frac{E_0 - T}{\sigma}\right) \times (M - C_s \times (E_0 - T))
\]  

(4.1)

\[
\text{Erf}(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} e^{-\frac{(x')^2}{2\sigma^2}} \, dx'
\]  

(4.2)

where \(T\) is the inflection point, \(\sigma\) is the gradient of the inflection point, \(M\) is the mean flux in the region fitted, and \(C_s\) is a slope related to charge sharing, an effect discussed below.

Analysing the shape of the S-curve can reveal information about the underlying interaction mechanisms. As an example, in the case where a photon interaction occurs at a distance from the center of the strip, the charge cloud generated by the incoming photon will be shared between two adjacent strips rather than been fully collected by a single channel. As a result of this charge sharing, the S-curve is not perfectly flat, but displays a slope as shown for the realistic S-curve in Figure 4.4 towards lower energies.

Another effect revealed in the S-curve is that of electronic noise. The S-curve departs from a sharp step function via the appearance of a gradient, whose inclination relates to the Equivalent Noise Charge (ENC). The ENC is the amount of charge required at the input of the electronic chain to generate the same variation in signal at the comparator level [27], and is defined as:

\[
\text{ENC} = \frac{\text{noise output voltage}}{\text{signal output voltage for an input of one electron}}.
\]

ENC can be used to quantify the spectral resolution of single-photon-counting detectors, and is a quantification of the noise after shaping of the signal. Detector capacitance, reverse biases and pre-amplifier and shapers settings are all variables influencing the ENC. The value of ENC for a detector can be determined by fitting the gradient of the sharp rising in the S-curve and is reported in units of electrons. As each electron-hole pair created in CdTe requires an energy of 4.43 eV at room temperature [27, 28], it can be converted in user-friendly eV units. An example of a 2 keV ENC...
4.1. Primary characterization

is depicted in Figure 4.4 as the magenta dotted line for a single strip and as the solid green line for a multi-strip sensor.

4.1.4. Bias voltage

In the following, the effect of bias on charge collection is analyzed through threshold scans and their resulting S-curves. Sensors TS01-S and TS02-O were investigated using 25.51 keV X-rays from a silver (Ag) fluorescence source. In between each scan the bias was set to 0 V for 10 seconds and then to the desired voltage. The acquisition time for each threshold step in each scan was one second. In order to optimize for the low energy and low flux environment as well as charge carrier collection time, the selected detector settings were high-gain settings. See section 4.1.5 and Table 4.1 for a description of the pre-amplifier and shapers settings. A flow chart of the experimental method is presented in Figure 4.5.

As discussed earlier, the applied bias influences the drift velocity and therefore the time required to collect the charge carriers and thus the quality and efficiency of the signal. A careful selection of the appropriate bias is therefore crucial to the optimal functioning of the detector system. The results presented in this section as well as the results of the IV-curves of Section 4.1.1 were used to determine the optimal bias settings.

Displayed in Figure 4.6 are the results of the threshold scans performed for both, TS01-S (a) and TS02-O (b), sensors. The bias ranged from 300 V to 900 V and -100 V to -400 V for the TS01-S and TS02-O sensors respectively. Data obtained from each scan was fitted with the S-curve Equation 4.1 and the resulting inflection point trend is shown in Figure 4.7. The FWHMs of each S-curve is displayed as the error bars at each bias setting.

Both of the sensors portrayed different behaviors with respect to bias increase. Whereas the baseline noise amplitude of the TS01-S sensor increased with increasing bias to the point of encompassing the charge signal, the TS02-O noise remained constant throughout the bias changes. A common effect to both sensors was the shift in S-curve, and therefore inflection point. However, this shift differed in magnitude and direction. The TS01-S inflection point trend was away from the noise baseline following its spreading, causing a continuous loss of charge collected and a decrease in the quality of the threshold scans. From a bias of 700 V and above, the threshold scan fit quality was drastically reduced as it was approaching the diode breakdown visible in the IV
Figure 4.5. Flow chart of the experimental method followed to determine the optimal bias voltage for each sensor.
4.1. Primary characterization

Figure 4.6. Effect of bias voltage on threshold scan for sensors TS01-S (a) and TS02-O (b).
Figure 4.7. Effect of bias voltage on inflection point and FWHM for sensors TS01-S (a) and TS02-O (b).
4.1. Primary characterization

profile in Figure 4.2(a). On the other hand, the TS02-O trend was towards the baseline noise up to -350 V. Then it incurred a sudden collapse of the signal at a bias of -400 V, consistent with the start of a breakdown shown in Figure 4.2(b). The charge sharing remained constant across the bias range.

Together, the IV analysis combined with the bias analysis of both sensors indicate that the optimal working bias is 400 V for the TS01-S sensor and -250 V for the TS02-O sensor.

4.1.5. Detector settings

The ENC, and therefore the shape of the S-curve, are affected by the detector settings. Settings studied were that of the pre-amplifier and both shapers as described in Section 3.2 and Figure 3.4. For the measurements presented here, the detector exposure time was 500 milliseconds for each step in the threshold scans, and the biases of the sensors were set at 400 V for TS01-S and -250 V for TS02-O. A flow chart of the experimental method is presented in Figure 4.8.

As discussed in Section 3.2, the gain of the pre-amplifier was controlled by varying the voltage difference across the feedback capacitor which also affected the shaping time of the signal and thus the gain.

Three preferred settings have been defined for MYTHEN as high-gain, fast and standard pre-amplifier and shapers settings [50]. A small feedback capacitor setting implies a large gain, which is equivalent to a long shaping time of the signal, and is the ideal setting for a low energy experiment. A large gain allows for the full collection of the electron-hole pairs created, but limits the dynamic range available for X-ray imaging. This setting will, from here on, be referred to as high-gain setting. A large feedback capacitor setting implies a small gain, and thus a short shaping time, and is the ideal setting for high count rate environment. This settings will from here on be referred to as fast setting. The majority of applications criteria will be matched by the so-called standard setting. In this configuration, a balance is met for both the dynamic range and count rate.

For the analyses, a threshold scan was performed at each detector setting increment. Each resulting S-curve was then subsequently fitted using Equation 4.1. The results of the fits are shown in Figures 4.9, 4.10 and 4.11 for the pre-amplifier, the first and second
Chapter 4. Detector Characterization

Figure 4.8. Flow chart of the experimental method followed to determine the optimal detector settings for each sensor. The example shown is for the pre-amplifier. The same method was followed for the optimization both of the shapers.

It is evident that the gain setting of the pre-amplifier had a moderate impact on the inflection point of the S-curve, visible through the shift incurred by the inflection point of 3.45 %, equivalent to 10 DAC units for the TS01-S sensor and of 1.54 %, equivalent to 13 DAC units for the TS02-O sensor.

The effect of the first shaper’s gain on the threshold scan and the trend of the S-curve inflection point are shown in Figures 4.10 and 4.13 respectively. In the case of the

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![Graphs](1)

**Figure 4.9.** Effect of pre-amplifier settings on the threshold scan of the TS01-S (a) and TS02-O (b) sensors.
Figure 4.10. Effect of the first shaper settings on the threshold scan of the TS01-S (a) and TS02-O (b) sensors.
Figure 4.11. Effect of the second shaper settings on the threshold scan of the TS01-S (a) and TS02-O (b) sensors.
Figure 4.12. Inflection point trend of the pre-amplifier settings threshold scans of the TS01-S (red) and TS02-O (blue) sensors.

Figure 4.13. Inflection point trend of the first shaper settings threshold scans of the TS01-S (red) and TS02-O (blue) sensors.
4.1. Primary characterization

TS01-S sensor, a shift of 63 DAC units equivalent to 10.36 % is observed up to a shaper gain equivalent to 430 DAC units. Beyond a gain of 430 DAC units, the detector is reaching an upper limit with very high-gain settings, drastically reducing the quality of the S-curves. As for the TS02-O electron collecting sensor, it incurs a lesser total shift of 38 DAC units or 6.77 %. Between the settings of 200 to 400 DAC units, the shift is linear. From a setting of 400 DAC units onwards the inflection point trend is asymptotic.

As shown in Figures 4.11 and 4.14, the second shaper had a very reduced effect on the shaping time and signal gain compared to the pre-amplifier and first shaper. The total fluctuation impact on the inflection point of the TS01-S S-curves is of 11 DAC units, equivalent to 3 %. As for sensor TS02-O the S-curves are fluctuating within a range of 4 DAC units equivalent to 0.63 %.

Using a combination of the inflection point trend shown above as well as a visual optimization of the signal-to-noise ratio via an oscilloscope, the three settings have been selected and optimized for the MYTHEN CdTe system and summarized in Table 4.1.
Table 4.1. Summary of optimized sensors settings.

<table>
<thead>
<tr>
<th>Setting</th>
<th>TS01-S</th>
<th>TS02-O</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fast</td>
<td>pre-amp 50 DACu</td>
<td>pre-amp 50 DACu</td>
</tr>
<tr>
<td></td>
<td>shaper1 200 DACu</td>
<td>shaper1 100 DACu</td>
</tr>
<tr>
<td></td>
<td>shaper2 300 DACu</td>
<td>shaper2 380 DACu</td>
</tr>
<tr>
<td>Standard</td>
<td>pre-amp 100 DACu</td>
<td>pre-amp 100 DACu</td>
</tr>
<tr>
<td></td>
<td>shaper1 300 DACu</td>
<td>shaper1 300 DACu</td>
</tr>
<tr>
<td></td>
<td>shaper2 260 DACu</td>
<td>shaper2 260 DACu</td>
</tr>
<tr>
<td>High-gain</td>
<td>pre-amp 200 DACu</td>
<td>pre-amp 200 DACu</td>
</tr>
<tr>
<td></td>
<td>shaper1 400 DACu</td>
<td>shaper1 400 DACu</td>
</tr>
<tr>
<td></td>
<td>shaper2 260 DACu</td>
<td>shaper2 260 DACu</td>
</tr>
</tbody>
</table>

4.2. Energy calibration and ENC

Measurements of the energy calibration and resolution of a new sensor are ideally performed in a monochromatic beam of energy resolution \( \Delta E/E \) superior to that of the detector system under investigation. The energy resolution of the Material Science beamline at the SLS is \( 1.4 \times 10^{-4} \) \([2]\) and thus well suited to this purpose.

The purpose of an energy calibration is to provide a mapping between the DAC units of the comparator into end-user friendly keV units. In order to achieve this, threshold scans were performed at multiple energies. Each threshold scan was then fitted with the S-curve Equation 4.1. The inflection point of the fit was then used in the calibration and fitted assuming a linear relationship, whereas the FWHM provided the ENC. The variables of the calibration’s linear fit were subsequently used to convert DAC units into keV. A flow chart of the experimental method followed is presented in Figure 4.15.

A schematic of the experimental setup as well as a photograph are shown in Figure 4.16. The monochromatic beam was focused onto a glass rod in order to elastically scatter the photon beam and produced a flat field onto all mounted sensors simultaneously.

In this study, three different sensors were studied at the X04SA beamline of the SLS at separate points in time. Sensors TS01-S and TS04-O were studied with monochromatic beam of energies 20 keV, 25 keV, 30 keV and 35 keV and standard pre-amplifier and shapers settings. The TS03-S sensor was calibrated with energies of 25 keV, 27 keV, 32 keV and 37 keV, calibrating both standard and fast pre-amplifier and shapers settings. The energies were carefully selected to surround the emissions and absorption...
4.2. Energy calibration and ENC

Figure 4.15. Flow chart of the experimental method followed to determine the energy calibration and ENC for each sensor.
Figure 4.16. Photograph and schematic of the experimental setup for the energy calibration measurements.
energies of both the Cd and Te. Cd has an emission energy of 23.17 keV and absorption energy of 26.7 keV, whereas Te emission and absorption energies are at 27.47 keV and 31.8 keV respectively [7].

Table 4.2 summarises the acquisition times, bias voltages applied and the gain settings used for each threshold scan and sensors.

The threshold scans for all four energies, including their fits, as well as the resulting calibration for sensor TS01-S for a sample channel with typical behavior are displayed in Figure 4.17. The threshold scans are here normalized as different fluxes were available for each selected energy, thus limiting a visual comparison of the resulting fits. The error-bars in the energy calibration are the FWHM of the fitted S-curves, and are the relevant parameter to calculate the ENC. In Figure 4.18 the histograms of the ENC distribution across all channels and for each of the energies are shown, and were each fitted with a Gaussian. The means of the Gaussians are the data points in Figure 4.18(e), and the FWHMs of the Gaussians are the error-bars. An energy of 35 keV was at the upper limit available at the Material Science beamline, SLS. The flux was, therefore, greatly reduced and the beam energy resolution degraded. Both factors were visibly impacting on the ENC of the sensor. Nevertheless, the energy calibration of the sensor remains linear in the energy range studied.

Table 4.2

<table>
<thead>
<tr>
<th>Sensor</th>
<th>Energy</th>
<th>Bias Voltage</th>
<th>Acquisition time</th>
<th>Settings</th>
</tr>
</thead>
<tbody>
<tr>
<td>TS01-S</td>
<td>20, 25, 30 and 35 keV</td>
<td>400 V</td>
<td>1 s</td>
<td>std</td>
</tr>
<tr>
<td>TS04-O</td>
<td>20, 25, 30 and 35 keV</td>
<td>-137 keV</td>
<td>1 s</td>
<td>std</td>
</tr>
<tr>
<td>TS03-S</td>
<td>25 and 27 keV</td>
<td>-300 V</td>
<td>500 ms</td>
<td>std / fast</td>
</tr>
<tr>
<td></td>
<td>32 keV</td>
<td>-300 V</td>
<td>1 s</td>
<td>std / fast</td>
</tr>
<tr>
<td></td>
<td>37 keV</td>
<td>-300 V</td>
<td>5 s</td>
<td>std / fast</td>
</tr>
</tbody>
</table>
Figure 4.17. Normalised threshold scans and S-curve fits for energies of 20 keV, 25 keV, 30 keV and 35 keV for sensor TS01-S (a) and the corresponding energy calibration (b) for standard pre-amplifier and shapers settings. The fitted S-curve of the threshold scans are used for the energy calibration. The errorbar in the energy calibration are the FWHM of the fitted S-curves.
4.2. Energy calibration and ENC

Figure 4.18. Sensor TS01-S ENC distribution (all strips) measured as a function of X-ray energy using standard pre-amplifier and shapers settings. The mean gaussian fit of the histogram is the ENC and the FWHM of the fit is the ENC’s errorbar as used in Figure (e).
Table 4.3. Summary of ENC for all sensors and energies studied.

<table>
<thead>
<tr>
<th>Sensor</th>
<th>20 keV</th>
<th>25 keV</th>
<th>30 keV</th>
<th>35 keV</th>
</tr>
</thead>
<tbody>
<tr>
<td>TS01-S (std)</td>
<td>2.42 ± 0.1 keV</td>
<td>2.71 ± 0.06 keV</td>
<td>3.12 ± 0.11 keV</td>
<td>3.40 ± 0.28 keV</td>
</tr>
<tr>
<td>TS03-S (std)</td>
<td>2.44 ± 0.05 keV</td>
<td>2.50 ± 0.06 keV</td>
<td>2.87 ± 0.07 keV</td>
<td>2.65 ± 0.09 keV</td>
</tr>
<tr>
<td>TS03-S (fast)</td>
<td>2.46 ± 0.05 keV</td>
<td>2.52 ± 0.07 keV</td>
<td>2.93 ± 0.15 keV</td>
<td>2.97 ± 0.12 keV</td>
</tr>
</tbody>
</table>

linear up to at least 35 keV. The ENC for each of the 14 individual channels available for this measurement is shown in Figure 4.20. As can be seen, the ENC for 35 keV spreads across 3.5 keV. The spread is related to the quality of fit of the threshold scan S-curve, and is affected by a reduced charge signal due to the reduced flux available.

TS03-S was the final sensor calibrated with energies of 25 keV, 27 keV, 32 keV and 37 keV. The respective threshold scans and calibration fits are shown in Figure 4.21 and 4.22 for standard and fast settings respectively. As expected from the discussion in Section 4.1.5, each threshold scan is shifted towards the baseline noise for fast settings with respect to standard pre-amplifier and shapers settings due to the reduced gain. In both cases, the energy calibration remains linear in the studied range. However, there is an increase in the ENC for fast settings at the top of the energy range studied, probably due to a shorter shaping time increasing the noise.

In conclusion, all sensors are displaying a linear energy calibration up to at least 35 keV. A summary of the ENC for each sensor and gain setting combination can be found in Table 4.3.
4.2. Energy calibration and ENC

Figure 4.19. Normalised threshold scans and S-curve fits for energies of 20 keV, 25 keV, 30 keV and 35 keV for sensor TS04-O (a) and the corresponding energy calibration (b) for standard pre-amplifier and shapers settings. The fitted S-curve of the threshold scans are used for the energy calibration. The errorbar in the energy calibration are the FWHM of the fitted S-curves.
Figure 4.20. ENCs for all strips for energies of 20 keV, 25 keV, 30 keV and 35 keV for sensor TS04-O for standard pre-amplifier and shapers settings.
4.2. Energy calibration and ENC

Figure 4.21. Normalised threshold scans and S-curve fits for energies of 25 keV, 27 keV, 32 keV and 37 keV for sensor TS03-S (a) and the corresponding energy calibration (b) for standard pre-amplifier and shapers settings. The fitted S-curve of the threshold scans are used for the energy calibration. The error-bar in the energy calibration are the FWHM of the fitted S-curves.
Figure 4.22. Normalised threshold scans and S-curve fits for energies of 25 keV, 27 keV, 32 keV and 37 keV for sensor TS03-S (a) and the corresponding energy calibration (b) for fast settings. The fitted S-curve of the threshold scans are used for the energy calibration. The error-bar in the energy calibration are the FWHM of the fitted S-curves.
4.2. Energy calibration and ENC

Figure 4.23. Distributions of all strips ENCs for energies of 25 keV, 27 keV, 32 keV and 37 keV for sensor TS03-S for standard pre-amplifier and shapers settings. The mean Gaussian fit of the histogram is the ENC and the FWHM of the fit is the ENCs errorbar as used in (e).
Figure 4.24. Distributions of all strips ENCs for energies of 25 keV, 27 keV, 32 keV and 37 keV for sensor TS03-S for fast settings. The mean Gaussian fit of the histogram is the ENC and the FWHM of the fit is the ENCs errorbar as used in (e).
4.3. Count rate and dead-time

An essential attribute of an X-ray detector for use with intense X-rays sources such as a synchrotron is the count rate capability, which describes the ability of the detector system to distinguish between two photons whose arrival times are very close. For these photons to be correctly counted, the analogue signal of the first photon must return below the comparator threshold prior to the rising of the next signal. Therefore, after each event is recorded, there is a time period during which the system cannot detect a new event which is referred to as dead-time. The system is inoperative for as long as the first pulse waveform remains above the threshold, and in the case of a second pulse arriving during that period, the dead-time is extended \[57\].

In a low flux environment, dead-time is rarely an issue as the pulses are temporally well separated. As the flux is increased, the time between pulses decreases and they gradually begin to overlap. This is commonly referred to as pile-up \[58\]. At very high flux, the extension of dead-time leads to paralysis, where an increasing impinging photon rate results in a lower observed count rate \[59\]. An ambiguity arises as to the number of true incoming photons from the observed photons count. A detector system displaying such ambiguity at very high count rate is called a paralizable detector \[60\]. The count rate behavior of such a detector can be described by \[59–61\]:

\[
N_{\text{out}} = N_{\text{in}} e^{-N_{\text{in}} \tau}
\]  

(4.3)

where \(N_{\text{out}}\) is the observed rate, \(N_{\text{in}}\) is the true photon rate and \(\tau\) is the effective dead-time parameters, which depends on the intrinsic detector response time and the spacing of X-ray pulses.

A theoretical example of the effect of high flux on the count rate of a paralizable system is shown in Figure 4.25. In red are the individual signal from impinging photons. In blue is the signal after amplification through pre-amplifier and shapers. The lower plot shows the output of the discriminator, i.e. the number of photons registered by the counter. In this example, only six out of 13 photons are counted. In the case of a threshold scan, this translates in a shift of the S-curve towards the baseline noise and the creation of a tail towards higher energy thresholds.

Count rate measurements of the TS03-S sensor were performed with standard and fast pre-amplifier and shapers gain settings using a 25 keV monochromatic beam of the Material Science beamline. A flow chart of the experimental method is presented in Figure 4.26.
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Figure 4.25. Schematic of the pile-up effect. In red are the individual photons impinging onto the sensor. In blue the signal after amplification through the pre-amplifier and shapers. The lower plot shows the discriminator output, i.e. the number of counts. 13 photons are impinging the sensor but only 6 are counted.

In order to vary the flux impinging onto the detector system, an EPICS (Experimental Physics and Industrial Control System) script was implemented to coordinate the filter combinations and shutter opening time. Table 4.4 is listing the available filters with their respective thicknesses. The filters were located towards the end of the beam path, before the slits and a MYTHEN module with a silicon sensor used as an incoming flux monitor (MIO). This detector system was selected as the reference flux monitor as it has been thoroughly characterized and its count rate calibration is well understood [62].

The MIO was placed below the beam and perpendicular to it, collecting the air scattered photons, whereas the CdTe detector system with TS03-S was placed front on. See Figure 4.27 for a schematic of the experimental setup.

The bias for TS03-S was rapidly cycled to zero and back to -300 V in between each flux increase. A threshold scan with acquisition time of one second per step was performed.

Table 4.4. List of available filters for the count rate measurement.

<table>
<thead>
<tr>
<th>Filter</th>
<th>Thickness</th>
</tr>
</thead>
<tbody>
<tr>
<td>Si - 50 μm</td>
<td>Si - 100 μm</td>
</tr>
<tr>
<td>Si - 1600 μm</td>
<td>Si - 2400 μm</td>
</tr>
</tbody>
</table>
4.3. Count rate and dead-time

Figure 4.26. Flow chart of the experimental method followed to determine the maximum count rate and dead-time of the sensor.

Figure 4.27. Experimental setup of the count rate and dead-time study.
Chapter 4. Detector Characterization

at every selected flux. Figure 4.28 shows the threshold scans for each chosen filter combination for standard (a) and fast (b) pre-amplifier and shapers settings. In both figures the red scan is the reference threshold scan performed at the lowest flux, the black scan is performed in the proximity of the onset of paralysis, and the green scan is the result of the threshold scan performed at the highest selected flux. The appearance of a tail in the high threshold region for high fluxes is accounting for the lost counts at lower thresholds due to pile-up.

Each threshold scan was fitted with an S-curve as per Equation 4.1. The inflection point evolution for the sample channel at standard and fast pre-amplifier and shapers settings is shown in Figure 4.29. Up to filter combination (index) 11, corresponding to a flux of average $1.4 \times 10^5$ ph/strips and equivalent to $2.3 \times 10^5$ ph/mm$^2$, the inflection point shifts by less than 1% for both standard and fast pre-amplifier and shapers settings. Above this flux, which was the onset of pile-up, the shift increased to 3.5% and 2.8% for standard and fast settings pre-amplifier and shapers respectively.

In order to find the maximum count rate and dead-time of the system, the baseline noise was fitted with a Gaussian as shown in Figures 4.30 (a) and (b) for standard and fast pre-amplifier and shapers settings respectively. The accurate determination of the baseline noise width requires the threshold scan to encompass the entire baseline noise starting below a threshold equivalent to 0 mV, here set at 460 DAC units in order to process charge carriers of either polarity. The result of the Gaussian fit of the noise as well as the selected threshold for further analyses are shown. The selected threshold for the count rate analyses is 5σ away from the mean, within the charge sharing region, and as close as possible to the threshold at half the energy of the incoming photon.

In Figure 4.31, the detected photon count was the one registered by the detector, whereas the incoming photon count was the true and absolute count calculated via the use of the MIO. In order to obtain the true and absolute incoming photon count, the MIO detector system performed an image acquisition of a duration of 100 seconds with the comparator level set at 12.58 keV, which was half the incoming photons’s energy, at each selected flux. The maximum total count of air scattered photons recorded during the acquisition time at the highest selected flux was $4.5 \times 10^4$ photons, which remained well within the linear count region of the detector system as discussed in [51]. Combining the MIO counts, together with the TS03-S count rate study for the first 10 fluxes allowed the absolute incoming photon flux to be calculated.

The number of photons impinging the CdTe system front on for the first 10 fluxes was low enough to remain within the linear count capability of the electronics. This was
4.3. Count rate and dead-time

Figure 4.28. Threshold scans performed with sensor TS03-S with increasing flux of 25 keV monochromatic photon beam for standard (a) and fast (b) settings. Red scan is the reference scan performed at the lowest flux. The green scan is the final scan performed at the highest flux.
Figure 4.29. Trend of the inflection point of the sample channel threshold scans fitted with the S-curve equation \( f(x) \) for each selected flux for the count rate and dead-time analyses for standard settings (a) and fast settings (b) for the pre-amplifier and shapers.
4.3. Count rate and dead-time

Figure 4.30. Reference threshold scan performed with low flux of 25 keV monochromatic photon beam for standard (a) and fast (b) settings. Baseline noise is fitted with a Gaussian. The green point is $5\sigma$ away from the noise peak.
therefore the true and absolute photon count for each individual strip. To obtain the absolute beam flux a linear fit to the first 10 seconds fluxes of the recorded counts was performed. Gradient and y-intercept of the fit were then used to calibrate the MIO counts to be true and absolute for the strip under investigation. The resulting calibrated MIO is the x-axis in Figure 4.31.

The fitting of the count rate and shaping time data was performed on a strip basis. Figure 4.31 shows the standard and fast pre-amplifier and shapers settings results for a sample channel. The blue and red linear fits show the result of the calibration of the MIO and thus the resulting linear relationship between incoming and detected counts at low fluxes.

Both standard and fast pre-amplifier and shapers settings were fitted with Equation 4.3. This fit was performed for each channel at the 5σ threshold away from the noise baseline. The distribution of the effective dead-time for all strips is shown in Figure 4.32 for standard and fast pre-amplifier and shapers settings. The resulting histograms were fitted with a Gaussian, where the mean value of the Gaussian fit is the overall effective dead-time of the system, which is $1.98 \pm 0.39\mu s$ for standard and $1.63 \pm 0.51\mu s$ for fast pre-amplifier and shapers settings.
4.3. Count rate and dead-time

Figure 4.32. Distributions of shaping time for standard (a) and fast (b) settings. They are fitted with a Gaussian. The mean of fit is the dead-time quoted with the FWHM as its error.
Chapter 4. Detector Characterization

Table 4.5. Effective dead-time and maximum count rate for Sensor TS03-S.

<table>
<thead>
<tr>
<th></th>
<th>Standard settings</th>
<th>Fast settings</th>
</tr>
</thead>
<tbody>
<tr>
<td>Effective dead-time</td>
<td>1.98 ± 0.39 µs</td>
<td>1.63 ± 0.51 µs</td>
</tr>
<tr>
<td>Maximum count rate</td>
<td>0.78 ± 0.17 MHz/mm\textsuperscript{2}</td>
<td>1.11 ± 0.25 MHz/mm\textsuperscript{2}</td>
</tr>
</tbody>
</table>

The maximum count rate for each strip before paralysis of the detector and readout system combination begins is the maximum of the fit in Figure 4.31. Figure 4.33 shows the distribution of the maximum count rate for all strip for standard and fast pre-amplifier and shapers settings. The histograms were fitted with a Gaussian and the resulting mean value is the maximum count rate of the system, which is 0.78 ± 0.17 MHz/mm\textsuperscript{2} for standard and 1.11±0.25 MHz/mm\textsuperscript{2} for fast pre-amplifier and shapers settings.

A summary of the dead-time and maximum count rate of the TS03-S MYTHEN CdTe sensor can be found in Table 4.5.

4.4. Summary

In summary, during the primary detector characterization IV-curves were performed and showed expected diode-like behavior for the Schottky sensors and semi-linear behavior for the ohmic contacts sensors. A series of line scans highlighted some tellurium inclusions within the CdTe sensors. Their impact on the functionality of the strip detector was minimal and easily rectified by the use of a flat field. Optimal working bias voltage were also determined for all sensors, followed by the analysis of the effect of pre-amplifier and shapers on the signal collected as well as optimization of the preferred settings for CdTe sensors. The selected pre-amplifier and shapers settings optimized for the remainder of this thesis are listed in Table 4.1. Next, energy calibration studies were performed for standard and fast pre-amplifier and shapers settings, which all demonstrate a linear behavior up to energies of 37 keV. From the data obtained and fitted for the energy calibrations, one could extract the FWHM and thus calculate the ENC for each sensor at each selected energy, which are summarised in Table 4.3. The last characterization measurement was a count rate study. The resulting effective dead-time of the system is 1.98 ± 0.39 µs and 1.63 ± 0.51 µs for standard and fast pre-amplifier and shapers settings respectively. The maximum average count rate
4.4. Summary

Figure 4.33. Distributions of maximum count rate for standard (a) and fast (b) settings. They are fitted with a Gaussian. The mean of fit is the maximum count rate quoted with the FWHM as its error.
across all strips is $0.78 \pm 0.17 \text{ MHz/mm}^2$ per strip for standard and $1.11 \pm 0.25 \text{ MHz/mm}^2$ for fast pre-amplifier and shapers settings.
It has been widely reported in the literature \cite{35, 36, 40, 63, 65} that CdTe detectors suffer degradation, commonly referred to as polarization. Polarization can be induced either by the presence of bias voltage or intense irradiation and can adversely affect the detector’s ability to perform. Earlier, in Section 2.3 a theoretical background for the underlying mechanisms of each type of polarization was discussed. The experimental results of both effects will be presented, analyzed and discussed together with a high count rate stability study, which is aimed at establishing the flux and temporal limits within which the detector system remains fully operational.

5.1. Bias induced polarization

In order to examine the stability of the sensor under prolonged biasing period, the sensor TS03-S was continuously biased for up to respectively 10 and 60 minutes. During these measurements a focused 25 keV monochromatic beam was scattered off a glass rod, producing a broad low flux beam which covered the entire surface of the sensitive area. Threshold scans were performed at regular intervals in order to verify if a degradation in charge collection could be observed. The acquisition time for each
Chapter 5. Polarizations Studies

threshold scan step was 100 milliseconds, and the bias polarization measurement was repeated for biases of -150 V, -300 V, -450 V and -600 V. A 10 second reset power cycle was performed at the start of each measurement and before each bias change. A flow chart of the experimental method followed is presented in Figure 5.1.

For each of the bias settings, a reference threshold scan was performed at the standard and fast pre-amplifier and shapers settings on a sample channel. The results obtained are presented in Figure 5.2. The black highlighted thresholds are 5σ away from the noise peak, resulting from the baseline noise Gaussian fits, whereas the magenta (-150 V), cyan (-300 V), pink (-450 V) and yellow (-600 V) thresholds are the inflection points resulting from the S-curve fits.

As the reference threshold scans for biases between -300 V and -600 V are similar, this shows that all the charge carriers were collected for these selected biases. The similarity in the reference scans also demonstrate that a power cycle of 10 seconds did reset the detector to its original performance, circumventing any potential polarization effects. However, at a reduced bias of -150 V, the sensor was not fully depleted, thus not collecting all of the charge cloud, resulting in a shift of the threshold scan with respect to that of the other selected biases.

The threshold scans performed once a minute over a period of 10 minutes for a bias of -300 V, with standard and fast pre-amplifier and shapers settings, are shown in Figure 5.3. The fitted inflection point and 5σ thresholds from Figures 5.2 are used in combination with the threshold scan in Figure 5.3 to determine the stability of the system. As can be seen in Figures 5.4, the count capability of both thresholds remains stable for biases between -300 V and -600 V. However, at a bias of -150 V, polarization of the sensor is immediately obvious and the detection efficiency decreases by 80% within 10 minutes. At this reduced bias, the electric field shift discussed in Section 2.3 due to the space region created by hole detrapping at the anode, is expected to affect the detector more rapidly than at higher biases. At higher biases, the sensor is depleted beyond the thickness of the sensor, increasing the time before which the electric field at the cathode reaches negligible values.

The bias stability measurement was extended up to 60 minutes for a bias of -300 V with scans performed at five minute intervals. Figure 5.5 displays the resulting threshold scans of the sample channel. The red threshold scan was the reference scan performed at the start of the measurement. A degradation in threshold scan is clearly visible resulting from loss of counts, however no gain loss, thus, no shift in energy for the inflection point of the S-curve is noticeable. This is indicative of the complete loss of
5.1. Bias induced polarization

Figure 5.1. Flow chart of the experimental method followed to study the bias induced polarization.
Figure 5.2. Reference threshold scan at $t = 0$ min for a bias voltages of -150 V (black), -300 V (blue), -450 V (red), -600 V (green) with standard settings (a) and fast settings (b). The black thresholds are the thresholds 5σ away from the noise peak. The magenta (-150 V), cyan (-300 V), pink (-450 V) and yellow (-600 V) thresholds are the inflection points from the respectively fitted S-curves.
5.1. Bias induced polarization

Figure 5.3. Threshold scan resulting from a constant biasing period up to 10 minutes for a bias voltage of -300 V. (a) Resulting scans for standard settings. (b) Resulting scans for fast settings. The red dotted threshold scan is the reference scan performed at the start of the stability measurement.
Chapter 5. Polarizations Studies

Figure 5.4. Stability of 5σ threshold (a) and inflection point (b) for standard settings and (c) and (d) for fast settings as highlighted in Figure 5.2 under constant bias for bias voltages of -150 V (black), -300 V (blue), -450 V (red) and -600 V (green).
charge from an individual photon rather than the partial loss of charge from multiple photons interacting in the detector.

As demonstrated in Figure 5.6, the count efficiency over time for both selected thresholds remained relatively stable for up to 20 minutes. After this time the count capability decreased to 50% within the following 15 minutes. The count efficiency settled at 23% of the nominal count rate, on average across all channels, at the end of the measurement. The MYTHEN CdTe system has exceeded expectations and remained operational for up to 60 minutes.

These results confirm that as expected, the bias polarization is dependent on the bias applied. Increasing the bias increases the time during which the sensor remained stable. The increased bias implies an increased drift velocity, which increases the lifetime of the charge carriers. It also over extends the depletion region beyond the limits of the sensor bulk, thus, extending the time available before the shift in electric field impacts the charge collection. Nevertheless, with a 500 μm thick CdTe Schottky sensor biased at -300 V and at an incident photon beam energy of 25 keV, experiments of duration less than 20 minutes can be performed without any initial biasing period required. For longer experiments it is recommended that the bias be applied up to
5.2. Radiation induced polarization

The second polarization mechanism investigated was radiation induced polarization. In order to test the sensors under high fluxes of $1 \times 10^9$ ph/s/mm$^2$ (int 1), $2 \times 10^9$ ph/s/mm$^2$ (int 2) and $5 \times 10^8$ ph/s/mm$^2$ (int 3) a monochromatic 25 keV beam was vertically collimated to 500 $\mu$m. At the end of a pre-defined period of time the threshold scan was performed. The waiting period prior to the start of the threshold scan was increased from 0 to 30 minutes in 30 second intervals. A 10 second reset power cycle was performed at the start of each measurement and before each bias change. When performing the threshold scan the flux was reduced to $8 \times 10^3$ ph/s/mm$^2$ in order to remain comfortably within the rate capability of the read-out system. This high radiation measurement was repeated for biases of -300 V and -450 V (flux of $1 \times 10^9$ ph/s/mm$^2$ only). All threshold scans were performed with fast pre-amplifier and shapers settings as this gain setting was more suitable for rapid successive measurements, as discussed.
Table 5.1. Summary of bias induced polarization results for sensor TS03-S and standard settings.

<table>
<thead>
<tr>
<th>Bias</th>
<th>Test period</th>
</tr>
</thead>
<tbody>
<tr>
<td>-150 V</td>
<td>10 min (25 keV)</td>
</tr>
<tr>
<td></td>
<td>60 min (25 keV)</td>
</tr>
<tr>
<td>80% count efficiency loss</td>
<td>N/A</td>
</tr>
<tr>
<td>-300 V</td>
<td>stable</td>
</tr>
<tr>
<td></td>
<td>Stable up to 20 min</td>
</tr>
<tr>
<td></td>
<td>50% count efficiency loss</td>
</tr>
<tr>
<td></td>
<td>then asymptotes to-</td>
</tr>
<tr>
<td></td>
<td>wards 23% of original</td>
</tr>
<tr>
<td>-450 V</td>
<td>stable</td>
</tr>
<tr>
<td></td>
<td>N/A</td>
</tr>
<tr>
<td>-600 V</td>
<td>stable</td>
</tr>
<tr>
<td></td>
<td>N/A</td>
</tr>
</tbody>
</table>

in Section 4.1.5 A flow chart of the experimental method followed is presented in Figure 5.7.

A selection of the threshold scans performed at a bias of -300 V at each flux are shown in Figures 5.8(a)-(c) for the sample channel. The red threshold scan was the reference scan performed at the start of the irradiation period. As the non-normalized reference threshold scan all remained within statistical fluctuations of each other, it confirms that the radiation induced polarization affecting the sensors is only a temporary effect and has no impact on the long term behaviour of the sensor. A brief power cycle does reset the system to its original state.

An initial rapid decrease in count capability as well as a shift of the S-curve inflection point is presented in Figures 5.8. This behavior suggest both: a loss of the complete charge clouds of individual photons as well as a partial trapping of the charge carriers within the charge cloud generated by multiple photons may be occurring.

Displayed in Figure 5.9(a) is the trend for the inflection points from the S-curve fitted to the reference threshold scans of Figures 5.8(a)-(c). The trend confirms a rapid decrease of the count capability at the original inflection point for all three intensities which is
Figure 5.7. Flow chart of the experimental method followed to study the radiation induced polarization.
5.2. Radiation induced polarization

![Graphs showing beam induced polarization threshold scans](image)

(a) flux of $1 \times 10^9$ ph/s/mm$^2$
(b) flux of $2 \times 10^9$ ph/s/mm$^2$
(c) flux of $5 \times 10^9$ ph/s/mm$^2$

**Figure 5.8.** Beam induced polarization threshold scans performed with a monochromatic 25keV flux of $1 \times 10^9$ ph/s/mm$^2$ (a), $2 \times 10^9$ ph/s/mm$^2$ (b) and $5 \times 10^9$ ph/s/mm$^2$ (c) at a bias of -300 V. Threshold scans were performed with a reduced flux of $8 \times 10^3$ ph/s/mm$^2$. 

attributed to a decrease in the charge collected at the electrodes and, thus, a shift of the S-curve, typical of radiation induced polarization effect as explained in [2.3.2] and described in references [39, 40, 66] in the case of pixellated detector systems.

In regards to the threshold 5$\sigma$ away from the mean of the baseline noise, the resulting trend for all three intensities studied and a bias of -300 V is shown in Figure 5.9(b). An initial count loss within the first 5 minutes is visible, which then stabilizes between 50% and 70% of the original count rate, depending on the flux. As shown in Section 5.1, the efficiency at high photon rates remains more stable than at low photon rates. A high flux appears to have a beneficial effect on the overall loss of efficiency for a threshold close to half of the energy of the incoming photon, partially counteracting the effects of bias induced polarization.

The high flux irradiation measurement has been repeated for a flux intensity of $1 \times 10^9$ ph/s/mm$^2$ and a bias of -450 V. Figure 5.10 shows the resulting threshold scans, as well as the inflection point and 5$\sigma$ thresholds trends in Figure 5.11(a) and (b) respectively. Increasing the sensor bias reduces the likelihood of the radiation induced polarization affecting the sensor, as after a decrease in count over the first 15 minutes, the count efficiency at the inflection point stabilizes itself at 25% of the original count capability. The threshold 5$\sigma$ from the noise peak is demonstrating a linear decrease in count over the entire 30 minutes period down to 85% of the original count capability. As this decrease is linear, it can be corrected for during post processing.

All of the irradiation measurements, which were performed with fluxes of $5 \times 10^8$ ph/s/mm$^2$ and higher, showed a polarization effect impacting the CdTe sensor detection efficiency. This is evident in the threshold scans which exhibit a gradual shift towards lower energies and a decrease in detected counts. This polarization effect, however, remains temporary and can be circumvented by either lowering the flux, or power cycling the bias to the sensor. Increasing the bias of the sensor also improves the count rate stability of the system, as the drift velocity and lifetime of the charge carriers are increased, thereby reducing the probability of trapping, and thus charge loss.

### 5.3. High count rate stability

In order to examine the count rate stability, a high count rate of 600 kHz and 900 kHz per strip (equivalent to fluxes of $8.8 \times 10^7$ ph/s/mm$^2$ (intensity 1) and $13.2 \times 10^7$ ph/s/mm$^2$
5.3. **High count rate stability**

![Graph showing inflection points and 5σ threshold](image)

**Figure 5.9.** Trend of the inflection points (a) and the points 5σ away from the baseline noise (b) during an extended irradiation with a monochromatic 25keV flux of $1 \times 10^9$ ph/s/mm$^2$, $2 \times 10^9$ ph/s/mm$^2$ and $5 \times 10^8$ ph/s/mm$^2$. 
(intensity 2) respectively, which remained within the count rate capability limits of the system, as discussed in Section 4.3, were selected. For this measurement rapid threshold scans were performed every 30 seconds for a period of up to 30 minutes, and were repeated for bias settings of -300 V, -450 V and -600 V. The system remained biased without reset power cycling for the entire 30 minutes period. A power cycle reset was, however, performed as each bias was applied. The 25 keV monochromatic beam was unfocused and vertically collimated to a width of 5 mm at the sensor by slits,
5.3. High count rate stability

Figure 5.11. Trend of the inflection points (a) and the points 5σ away from the baseline noise (b) and from the reference threshold scans in Figure 5.10 during an extended irradiation with a monochromatic 25keV flux of $1 \times 10^9$ ph/s/mm².
therefore covering 73% of the length of the strips and therefore avoiding the gold studs region discussed in Section 4.1.2. All threshold scans were performed with standard pre-amplifier and shapers settings as summarised in Table 4.1. A flow chart of the experimental method followed is presented in Figure 5.12.

Presented in Figure 5.13 is the reference threshold scans for all three biases performed at the start of the measurement. For both intensity and all three biases, the inflection point and $5\sigma$ thresholds are identical, indicating that at those biases all of the charge...
5.3. High count rate stability

![Figure 5.13](image)

**Figure 5.13.** Reference threshold scans for high count rate study for biases of -300 V (blue), -450 V (red) and -600 V (green) with a flux of 8.8 x10^7 ph/s/mm^2. The inflection point is highlighted in each scan with a magenta point. The threshold 5σs away from the baseline noise is highlighted by a black point in each scan.
carriers are collected. The tails at high energy in the threshold scans are expected due to the high flux, and are a sign of pile-up, consistent with the results presented in Section 4.3.

The reference threshold scan in red as well as the scans performed after 7.5 min (blue), 15 min (green), 22.5 min (cyan) and 30 min (black) for biases of -300 V, -450 V and -600 V respectively, are presented in Figures 5.14(a)-(c). For all three biases, a degradation in the quality of the S-curve is visible. There is a loss of count, and therefore charges, at the inflection point and an increase in charge collected in the charge sharing region as well an increase in the baseline noise amplitude. This behavior demonstrates consistency
Figure 5.15. Trend of the inflection point threshold during the high count rate study over a period of 30 minutes with standard settings. Three biases were studied: -300 V, -450 V and -600 V.

with the high irradiation polarization study in the previous section and a partial charge loss rather than a full photon count loss, supporting the hypothesis that the charge carriers are being individually trapped rather than an effect on the charge cloud as a whole.

For biases of -450 V and -600 V the inflection points threshold trends are very similar and constant, as shown in Figure 5.15. Any loss of count can be easily corrected for via post processing. On the other hand, the inflection point threshold count loss at -300 V is sharper during the first 10 minutes and then stabilizes after 20 minutes. This behavior does not require any post processing corrections. Imposing a waiting period of at least 20 minutes prior to any measurements is sufficient to counteract the count loss. Depending on the length of the measurement to be performed, higher bias can
Figure 5.16. Trend of the point 5σ threshold during the high count rate study over a period of 30 minutes with standard settings. Three biases were studied: -300 V, -450 V and -600 V.

be an improvement and benefit the overall detector performance in a high count rate environment.

The 5σ threshold trend in Figure 5.16 shows good agreement for both biases of -450 V and -600 V. During the 30 minutes stability measurement the count rate loss is less than 20%. At a bias of -300 V, the count rate remains stable for the entire period for intensity 2, whereas there is an increase in the collected charge after 15 minutes in the case of the first (lower) intensity studied. As seen in the bias induced polarization study and Figure 5.2, the baseline noise amplitude at a bias of -300 V is reduced compared to that of biases of -450 V and -600 V. The 5σ threshold is thus closer to the noise peak and towards lower energies. As the baseline noise amplitude increases over time, it absorbed the selected threshold, explaining the increase in counts after 15 minutes in Figure 5.16.
As end-users do not generally perform threshold trials during their experiments, but are more likely to set the discriminator threshold at half the energy of the incoming photons, it is recommended to use a beam energy of at least 25 keV in order to reduce the likelihood of a count increase due to a baseline noise amplitude increasing.

A summary of the results of the high count rate stability study can be found in Table 5.3.

<table>
<thead>
<tr>
<th>Bias</th>
<th>Inflection point</th>
<th>$5\sigma$ threshold</th>
</tr>
</thead>
<tbody>
<tr>
<td>-300 V</td>
<td>rapid loss for 10 min</td>
<td>int1: stable for 12 min</td>
</tr>
<tr>
<td></td>
<td>stable after 20 min at</td>
<td>then increase in count.</td>
</tr>
<tr>
<td></td>
<td>65% (int1) and 80% (int2) of original count efficiency</td>
<td>int2: stable during entire 30 min.</td>
</tr>
<tr>
<td>-450 V and -600 V</td>
<td>linear decrease in count over 30 min</td>
<td>linear decrease in count over 30 min</td>
</tr>
<tr>
<td></td>
<td>to 65% (int1) and 70% (int2) of original count</td>
<td>to 85% of original count for both int1 and int2</td>
</tr>
</tbody>
</table>

| 5.4. Summary |

In this Chapter the study and analysis of bias and radiation induced polarization effects have been presented as well as a stability study under high count rate. The results presented here demonstrate that the MYTHEN CdTe sensors are stable and fully functional for up to 20 min when over depleted. At a moderate flux, this is sufficient time to perform a various range of experiments such as powder diffraction patterns or computer tomography scans.

Radiation induced polarization effects were observed at incident fluxes of $5 \times 10^8 \text{ph/s/mm}^2$ or higher, which produced a reduction of gain and associated count losses. For a bias of -300V, at a threshold $5\sigma$ away from the baseline noise peak, a threshold close to that of half the energy of the impinging photons, it is observed that after an initial count loss during the first 3 minutes the detector system stabilises between 50% and 70% of the original count depending on the flux. When increasing the bias to -450 V, the count
loss is linear from the start of the measurement and declines to 80% of the original count after 30 minutes. The linearity and continuity of this count loss allows for simple post processing corrections to regain the lost counts if necessary. The effects resulting from radiation induced polarization are, thus, bias dependent and can be improved by increasing the bias voltage applied.

The stability of the system under a high count rate was also investigated, selecting count rates of 600 kHz and 900 kHz, which remain within the count rate limits of the system. Over a period of 30 minutes, the detector system demonstrated a slow and linear count loss of maximum 15% of the original counts. An effect which can easily be accounted for during post processing of the experimental data obtained.

In conclusion, the MYTHEN CdTe sensors show reliable performance under extended bias and high flux environment, with effects all reversible via a brief power cycle or flux reduction.
Conclusion and Further work

Meeting the ever-increasing demands for the next generation of X-ray imaging has been the prime motivation for the work reported in this thesis. As the thrust for embracing higher energy experiments has grown, limitations of silicon as a semiconductor have driven the need to introduce a new, higher Z, sensor material. In response to this need, the focus of this thesis has been the characterization of cadmium-telluride (CdTe) as a viable replacement for silicon as the sensor of choice for hybrid pixel detectors. Addressing the concerns of polarization in CdTe, which until now has prevented wide scale acceptance of the semiconductor, has required a deep understanding of the physical processes governing charge production and transport through semiconductors. A series of carefully planned experiments have been undertaken and the analysis of these confirm that both radiation and bias induced polarization effects can be managed. A novel MYTHEN system incorporating customized CdTe sensors has proven to be stable and reliable.
6.1. Primary characterization

Primary characterization such as current-voltage response has shown that Schottky type sensors behave similarly to diodes with a forward and a reverse bias polarity. Conversely the ohmic type sensors have demonstrated a semi-linear relationship between current and voltage. Tellurium inclusions within the sensor were identified in the linescan. In a strip detector these inclusions are of minimal impact and can be easily corrected for via flat field correction. Prior to the energy calibration and resolution study, the working bias for each detector and corresponding gain settings were optimized. The sensors remained well calibrated and the threshold-keV relationship found to be linear for energies up to 37 keV. The equivalent noise charge varied from $2.42 \pm 0.1$ keV for a 20 keV photon beam to $3.40 \pm 0.28$ keV for a 35 keV photon beam with standard settings for the pre-amplifier and shapers. Prior to the onset of paralysis, the maximum count rate for each strip is $0.78 \pm 0.17$ MHz/mm$^2$ for standard and $1.11 \pm 0.25$ MHz/mm$^2$ for fast pre-amplifier and shapers settings. This is equivalent to a dead-time of $1.98 \pm 0.39$ μs and $1.63 \pm 0.51$ μs for standard and fast pre-amplifier and shapers settings respectively.

6.2. Bias and radiation induced polarization

Bias and radiation induced polarizations have been discussed in the literature for more than a decade. The time frame reported is in the range of minutes for the bias induced polarization and seconds to minutes for the radiation induced polarization. In this thesis the effect observed in the stability study performed showed a bias dependent polarization. When depletion has been achieved, the Schottky sensor was affected within three minutes and the detector count rate was reduced to 20% after 10 minutes. Over-depletion reduced the count rate to 20% after 60 minutes. Individual charge carriers lost from multiple photon interactions in the sensor would result in a threshold-scan shift. As no such shift was observed, the photon count loss is concluded to be resulting from a loss of the complete charge cloud.

In order to study the effect of radiation induced polarization, three different fluxes ($1 \times 10^9$ ph/s/mm$^2$, $2 \times 10^9$ ph/s/mm$^2$ and $5 \times 10^8$ ph/s/mm$^2$) and three biases (-150 V, -300 V and -450 V) have been studied. Count rate loss as well as a shift in the threshold scans were observed, consistent with trapping of individual charge carriers and loss of photon counts. The results also revealed that a higher bias allowed the system
to remain functional for up to 30 minutes. Both polarization effects have a transient impact on the detection efficiency of the sensors. A brief power cycle allowed the sensors to resume normal performance.

The count rate stability of the detector system was also tested with count rates of 600 kHz and 900 kHz, which remained within the count rates capability limits of the system. This experiment showed bias dependent results. In the case of higher magnitude biases of -450 V and -600 V, the count capability decrease was slow and gradual, allowing for easily retrieval of the lost counts in post-data processing. A bias of -300 V initially results in a steep change followed by a plateau after 20 minutes.

Overall, the polarization effects observed on MYTHEN CdTe strip detector are temporary and show a slower impact than reported in the literature. Generally, a higher bias improved the stability of the detector. Depending on the type of experiments performed, an initial bias period should be applied to the sensor prior to the start of the measurement in order to fill the vacancies in the sensor bulk and stabilise the system.

6.3. Outlook

The body of the work presented in this thesis has demonstrated that the MYTHEN CdTe strip detector is a viable candidate as a new generation state-of-the-art X-ray imaging detector. The sensors have shown to have very promising stability under extreme conditions, as well as effects due to polarization that are all reversible via a simple and brief power cycle. All the experiments performed in this thesis were conducted at room temperature in a controlled 24 °C environment. It is potentially beneficial for the stability of the system to cool the sensor. Cooling the sensor has been reported to impact on the ionization time of the deep acceptor levels, thus improving the effects of polarizations. Overall, the sensors have shown very stable and linear performance within an energy range of 15 keV to 37 keV. Expanding the energy calibration up to an energy of 150 keV would allow coverage of a wider range of applications including medical imaging.

In order to fully utilise the energy range provided by the third generation synchrotron, a new hybrid system for powder diffraction could be comprised of two sensitive layers: a silicon sensor stacked over a CdTe sensor. Photons with an energy below or equal to 15 keV would interact predominantly within the first sensor thus utilizing the superior
Chapter 6. Conclusion and Further work

detection properties of silicon in that energy range. For photons with an energy higher than 25 keV the detection efficiency of silicon is greatly reduced. These photons would interact in the CdTe sensor with a higher quantum efficiency and travel through the Si layer largely unaffected as it would appear transparent to high energy photons. The synergy of such a hybrid system would allow the combination of the advantages of separated detector systems, while compensating each other’s limitations.

3D sensor architecture as proposed in [67,68] could potentially reduce the effect of bias and radiation induced polarizations occurring in CdTe detector systems. Unlike in planar detectors, where the electrodes are at the surface of the sensor bulk, in such a 3D assembly, the electrodes traverse the substrate in alternating pattern. Such a structure reduces the collection distance and therefore the charge collection time. The decreased distance between the electrodes also implies a lower depletion voltage and reduced leakage current. A reduction of the leakage current would be highly beneficial to the ohmic type sensors as they suffer a leakage current two orders of magnitude higher than Shottky diodes. A lower depletion bias may also have a positive impact on polarization effects, as it would allow for an extended plateau region in the IV response of the sensor and thus a wider over-depletion voltage range before breakdown. Furthermore, increasing the over-depletion voltage has shown to increase the mean free path of charge carriers in CdTe, reducing their probability of trapping and thus the effects of radiation induced polarization.


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List of acronyms

**ADC** - Analogue to digital converter

**Ag** - Silver

**Al** - Aluminium

**AMFPI** - Active Matrix Flat Panel Imagers

**ASIC** - Application Specific Integrated Circuit

**CCD** - Charge Coupled Device

**Cd** - Cadmuim

**CdTe** - Cadmium-Telluride

**CMOS** - Complementary metal-oxide semiconductor

**CT** - Computer Tomography
Chapter A. List of acronyms

DAC - digital to analogue converter

DQE - Detector Quantum Efficiency

ENC - Equivalent Noise Charge

ELS - Embedded Linux System

FWHM - Full Width Half Maximum

FPGA - Field Programmable Gate Array

GaAs - Gallium-Arsenid

In - Indium

IV - Current-voltage

LSF - Line Spread Function

Mo - Molibdenum

MYTHEN - Microstrip System for Time-resolved experiments

MCB - Module Control Board

PD - Powder diffraction

PET - Positron Emission Tomography

PSI - Paul Scherrer Institut

PSF - Point Spread Function

Pt - Platinum

Si - Silicon

SLS - Swiss Light Source

SNR - Signal to Noise Ratio
Te - Telluride

TFD - Thin Film Diode

TFT - Thin Film Transistor

X04SA - Material Science Beamline at the SLS

X05DA - Optics Beamline at the SLS

XRPD - X-ray powder diffraction

Z - atomic number
Publications
Characterisation of an electron collecting CdTe strip sensor using the MYTHEN readout chip


Abstract: MYTHEN is a single photon counting hybrid strip X-ray detector that has found application in x-ray powder diffraction (XRPD) experiments at synchrotrons worldwide. Originally designed to operate with hole collecting silicon sensors, MYTHEN is suited for detecting X-rays above 5 keV, however many PD beamlines have been designed for energies above 50 keV where silicon sensors have an efficiency of only few percent. In order to adapt MYTHEN to meet these energies the absorption efficiency of the sensor must be substantially increased.

Cadmium-Telluride (CdTe) has an absorption efficiency approximately 30 times that of silicon at 50 keV, and is therefore a very promising replacement candidate for silicon. Furthermore, the large dynamic range of the pre-amplifier of MYTHEN and its double polarity capability has enabled the characterisation of an electron collecting Schottky type CdTe sensor. A CdTe MYTHEN system has undergone a series of characterisation experiments including stress test of bias and radiation induced polarizations. The performance of this system will be presented and discussed.

Keywords: Hybrid detectors; Solid state detectors

1Corresponding author.
1 Introduction

MYTHEN is a single photon counting detector designed for powder diffraction experiments [1]. Powder diffraction synchrotron experiments have specific and challenging requirements: high spatial resolution is required to precisely determine diffraction maxima and infer micro-structural properties of the material. The type of atoms within a unit cell are defined by the intensity ratios of the peaks and the detector system requires therefore a large range in count rate capability. In this paper we therefore characterize the stability of the count rate at different fluxes.

Originally the semiconductor chosen for MYTHEN was silicon. The energy range with an efficiency above 50% for 320 \( \mu \text{m} \) Si is 3–16 keV. Increasing the silicon sensor thickness up to 1 mm extends the 50% efficiency limit to 23 keV. This modest improvement is accompanied by signal degradation due to increased charge sharing between strips. An alternative approach to extending quantum efficiency is to replace the semiconductor with a high Z material. Cadmium Telleuride (CdTe) is a suitable candidate due to its high quantum efficiency for photons of energy up to 100 keV even with a 500 \( \mu \text{m} \) thick sensor and room temperature operation [2].

In order fully cover an energy range from 5 keV up to 100 keV a MYTHEN system for powder diffraction could comprise two sensitive layers; a silicon sensor backed by a CdTe sensor.

In this study the semiconductor of the MYTHEN system has been replaced by CdTe. First the MYTHEN electronic chain and detector-sensor setup will be briefly described. In the next section the results of the detector characterisation, as well as investigations of polarization (bias and photon flux dependant) are presented.
2 Detector system description

2.1 The MYTHEN system

MYTHEN (Microstrip sYstem for Time-rEsolved experimeNts) is a single photon counting strip detector developed primarily for synchrotron radiation powder diffraction experiments. Each module consists of 10 chips with together 1280 channels wire bonded to the sensor. Each channel front end operates in parallel and comprises a charge sensitive preamplifier AC coupled to two shaping stages followed by a comparator, a pulse generator and a 24-bit counter [3]. The sketch of the front end chain is shown in figure 1.

The analogue chain can be adjusted to accommodate a wide range of applications by optimising with respect to low noise and high count rate. By comparing the signal amplitude with a threshold, the system is capable of performing energy discrimination, i.e. all electronic noise is rejected and the uncertainty on the number of counts is purely Poisson-like. The dual polarity of the system enabled by the capability to move the comparator threshold to both side of the analogue baseline allows collection of both holes and electrons. A more detailed description of the MYTHEN system can be found in [1].

2.2 CdTe sensor

To substantially extend the energy range a sensor with a higher atomic number is required. Cadmium-Telluride is a compound material with a high atomic number (48 and 52 respectively) and has a band gap of 1.51 eV at room temperature [4].

The CdTe semiconductors used for this study were manufactured by Acrorad Co., Ltd (Japan) [5]. The thickness of the sensor is 500 µm. It has 64 strips with a pitch of 100 µm and a length of 6.8 mm.

Figure 2 shows CdTe sensors bonded to a ceramic interposer via gold studs. The interposer is wire bonded to MYTHEN chips.

The result of a line scan of the system is displayed in figure 3. For this measurement a first prototype with the same geometry but ohmic contacts has been used. In order to perform this
B.1. Characterisation of an electron collecting CdTe strip sensor using the MYTHEN readout chip

Figure 2. Left: picture of a module with one silicon sensor and three CdTe sensors of the same geometry as the one tested is shown. Right: schematic of the CdTe sensor bonded via gold studs onto a ceramic interposer, which is wire bonded to a MYTHEN readout board.

Figure 3. Linescan of the sensor, performed with a 20 keV beam that was vertically constrained to 20 µm via precision slits.

measurement, a 20 keV monochromatic beam was vertically constrained to 20 µm using precision slits. The sensor was then vertically scanned in 20 µm steps in front of the beam. Two rows with reduced detecting efficiency are visible at each vertical extremity of the sensor. This are matching the positions of the gold studs used to connect the CdTe with the ceramic interposer. Smaller efficiency loss regions are spread out across the sensor. They are however sparse and affecting less than a region of 60 µm in height. The increase in counts towards the left side of the sensor is due to the beam geometry. The measurement in this study were performed with an untrimmed system. Therefore the count capability and threshold value at half of the energy of the incoming beam were not homogenised across the bonded channels, which results in count variations from channel to channel. For the planned powder diffraction application the intensity distribution along a strip is constant. The ineffective regions under the gold studs do not affect the measurement since these can easily be masked. Small inefficient regions can be corrected using flat field corrections.

In this study a sensor with a Al/CdTe/Pt contact configuration, forming a Schottky diode on the Al side and an ohmic contact on the Pt side, was characterised and tested. The IV-curve of the
Figure 4. IV-curve of the Schottky diode tested in this study. A waiting period of 60s was applied after each voltage step and prior to reading the leakage current. The inset plot shows the full range used for the IV-curve. The main plot is a zoom on the plateau region of the IV-curve. At −300 V the leakage current is about 30 nA. The abnormalities around 50 V are yet not understood.

Schottky sensor tested in this study is shown in figure 4. After each voltage step and prior to each leakage current measurement, a waiting time of 60s was applied. The IV-curve displays a typical diode like behavior with a strong forward bias increase and, at a reverse bias of −700 V, the start of a breakdown. At a bias of −300 V the leakage current was about 30 nA and stable in time.

3 Experimental results

The MYTHEN CdTe system was tested at the Material Science Beamline at the Swiss Light Source [6]. With an energy range from 5 to 40 keV it allows direct comparison of the original Si sensor with that of the CdTe sensor. The maximum flux provided is almost $10^{13}$ ph/s, thereby enabling high flux measurement and flux induced polarization tests.

3.1 Detector characterisation

Information regarding signal height, noise and charge sharing can be retrieved from threshold scans. Such a scan is obtained acquiring flat field images at variable threshold. For a noiseless system this would generate a sharp step function depending on pulse height, i.e. energy deposited by the incoming photon. The step function is then changed by the noise at the step and by the charge sharing at the plateau.

The gradient at the inflection point is proportional to the equivalent noise charge (ENC). This is the amount of charge or electrons required at the input of the electronic chain to generate the same variation in signal at the comparator level [7]. The charge cloud, after absorption of the photon in the sensor, will diffuse and spread within the sensor on its way to the electrodes and be shared between adjacent strips. The slope towards the base noise level is proportional to this charge sharing.

By fitting the S-curves with the equation

$$C = \text{Erf} \left( \frac{E_0 - T}{\sigma_{\text{enc}}} \right) \times (1 - C_s \times (E_0 - T)), \quad (3.1)$$

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one obtains the inflection point and sigma to perform the energy calibration of the detector [1]. The inflection point is used as the translation factor from DAC units to keV and the sigma is used to determine the electronic noise.

The sample S-curves as well as the results of the calibration of one sample channel in the energy range from 25 keV to 37 keV are respectively shown in figures 5(a) and 5(b). They properly fit Equation 3.1 showing that charge transport and collection follows the expected model without charge loss. The fit between all the inflection points is linear across the tested range, indicating a good linearity of the system.

The increase in noise counts around 510 DAC units for 32 keV and 37 keV compared to lower energies is due to an increase in exposure time. For the 25 keV threshold scan, an exposure time of only 100 ms was required and this had to be extended up to 5 s for the 37 keV threshold scan as the beam flux was highly reduced. The charge sharing plateau, located between the top of the S-curve and the start of the noise, is increased for the 32 keV and 37 keV. This is an indication of Cd and Te fluorescence.

The electronic noise, also called Equivalent Noise Charge (ENC), has been evaluated by fitting the S-curves for each energies using Equation 3.1. The resulting ENC for each energy is summarised in Table 1. Usually the minimum threshold should be at 10 times the noise, resulting in a minimum detectable energy of 24.2 keV.

Table 1. Summary of Equivalent Noise Charge (ENC) for incoming photon energies of 25 keV, 27 keV, 32 keV and 37 keV.

<table>
<thead>
<tr>
<th>Energy (keV)</th>
<th>25</th>
<th>27</th>
<th>32</th>
<th>37</th>
</tr>
</thead>
<tbody>
<tr>
<td>ENC (keV)</td>
<td>2.42 ± 0.024</td>
<td>2.49 ± 0.063</td>
<td>2.86 ± 0.124</td>
<td>2.67 ± 0.93</td>
</tr>
</tbody>
</table>

Figure 5. S-curves for energies 25 keV, 27 keV, 32 keV and 37 keV for Schottky diode sensor for a sample channel (left) and its corresponding energy calibration (right). There is a linear relationship maintained between DAC units and keV. Linear fit equation of the calibration is: Threshold [DAC] = 4.11 × E[keV] + 472.02.

B.1. Characterisation of an electron collecting CdTe strip sensor using the MYTHEN readout chip
Counts

Figure 6. Left: threshold scan resulting from an extended biasing period up to 2 hours for a bias voltage of $-300$ V. The black threshold scan is the reference scan taken at the start of the stability test without any waiting period applied. Right: count rate at a high threshold value of 17 keV (dashed lines) and low threshold value of 13 keV (solid lines) for four different biases (black $-150$ V, red $-300$ V, green $-450$ V, blue $-600$ V).

3.2 Bias induced polarization

It has been reported that CdTe suffers two type of polarization effects [8–13]. The first polarization type is a bias induced polarization and will be described here. The second type, a flux induced polarization, will be described in the next section.

In order to examine the stability of the sensor under extended biasing periods, the sensor was continuously biased up to two hours. For this test a focused 25 keV monochromatic beam was scattered off a glass rod, thereby covering the entire surface of the sensitive area with a moderately low flux. Threshold scans were performed at 5 minutes intervals for up to two hours in order to verify if a degradation in charge collection could be observed. This test was repeated for biases of $-150$ V, $-300$ V, $-450$ V and $-600$ V. During this stability measurement the sensor remained at a room temperature of 24°C and all threshold scans were taken with standard settings. A 10 s reset power cycle was performed between each bias change at the beginning of each delay scan.

The resulting threshold scans of the sample channel can be seen in figure 6(a) for $-300$ V. The black threshold scan is the reference scan taken at the start of the test without any waiting period. A degradation in threshold scan is clearly visible, however for $-300$ V no shift in energy for the inflection point of the Scurve is noticeable. This indicates more a loss of the complete charge of photons rather than a partial loss of charge of individual photons.

Figure 6(b) shows the count efficiency over time at two different threshold settings. The solid lines relate to a threshold of 13 keV, which is just above half the incoming energy, and the dashed lines to a higher threshold of 17 keV. Four different biases have been tested to examine any bias dependence.

At a bias of $-150$ V, the sensor polarizes instantly and loses all detection efficiency within the first two minutes. At a bias of $-300$ V, the detection efficiency is still decreasing but at a
more moderate rate. At the higher biases one can differentiate the efficiency loss of both threshold values. At low bias voltages (−150 V and −300 V), the effect seems to be more a total loss of charge for some photons, as the difference between high and low threshold is small. At high bias voltages (−450 V and −600 V), the polarization effect is more a partial loss of charge as seen from the difference of high and low threshold.

Overall, the bias polarization is dependant on the bias applied. At a higher bias of −600 V, the 500 µm Schotky diode tested here loses only 15 % of its efficiency in 2 hrs.

3.3 Flux induced polarization

The second polarization type is the flux induced polarization. In order to test the sensors under a high flux of $1 \times 10^9$ ph/s/mm$^2$ a monochromatic 25 keV beam was used. The 500 µm high beam impended on the sensor for a predefined period at the end of which a threshold scan was performed. The waiting period before the threshold scan was increased from 0 to 35 min. At first in 30 s intervals up to 5 min and then in 5 min intervals up to 35 min. A 10s reset power cycle was performed at the start of each delay scan and before each bias change. When performing the threshold scan the flux was reduced to $8 \times 10^3$ ph/s/mm$^2$ in order to remain comfortably within the rate capability of the readout system and not add a pile-up effect to the polarization. This test was repeated for biases of −150 V, −300 V and −450 V. During this flux induced polarization measurement the sensor remained at a room temperature of 24 °C and all threshold scans were taken with standard settings.

A selection of the threshold scans for the sample channel performed at a bias of −300 V is shown in figure 7(a). The red threshold scan is the reference scan taken at the start of the irradiation period without any waiting period applied. Between the first and second threshold scan after 30 s, a

![Figure 7. Left: threshold scan resulting from an extended high flux irradiation period up to 35 min for a bias voltage of −300 V. The red threshold scan is the reference scan taken at the start of the irradiation test without any waiting period applied. Right: count rate at a threshold value of 13 keV for three different biases (black −150 V, red −300 V, green −450 V).](image)
decrease in count efficiency as well as a shift in S-curve has been measured. Figure 7(b) depicts the count efficiency at a fixed threshold value of 13 keV over time for bias values of −150 V, −300 V and −450 V. Both figures indicate an initial rapid decrease in count capability as well as a shift of the S-curve inflection point. Indicating both a loss of the complete charge of some photons and for others only a partial loss of charge. After 15 min the count capability stabilises at a bias of −450 V and fluctuates between 80 % and 85 % of the initial count efficiency. At a bias of −300 V the count loss fluctuates between 5 % and 45 %.

Where the large fluctuations in the normalized number of counts come from is currently unclear. In the future we will study a potential recovery effect after removing the high photon flux. Comparing figures 6(b) and 7(b) (−300 V and −450 V), shows that the efficiency at high photon rates drops slower than at low photon rate. A high flux therefore is having a beneficial effect on the loss of efficiency.

3.4 High count rate stability

In order to examine the count rate stability, a high count rate of 600 kHz per strip (equivalent to a flux of $8.8 \times 10^7$ ph/s/mm$^2$), which is within the count rate capability of the system, was selected. For this measurement rapid threshold scan were performed every 30 s for a period of 30 min. This was repeated for bias settings of −300 V, −450 V and −600 V. The system remained biased without reset power cycling for the entire 30 min period. A power cycle reset was however performed after the bias was changed. The 25 keV monochromatic beam was unfocused and vertically constrained to 5 mm by slits. During this high count rate measurement the sensor remained at a room temperature of 24 °C and all threshold scans were taken with standard settings.

The result of the threshold scan for a bias of −300 V is shown in figure 8(a). A shift of the S-curve is visible over a period of 30 min. This indicates that the main effect is a partial loss of charge for individual photons. In figure 8(b) the count rate is displayed for the three different biases and two threshold values respectively equivalent to 12.5 keV and 17 keV. At an energy of 12.5 keV, which is half the energy of the incoming photon beam, the count rate remains stable for the length of the measurement. This is the crossing point of all S-curves in figure 8(a). At an energy of 17 keV, a count loss due to the shift in S-curve as seen in figure 8(a) is visible. This count loss remains however below 20 % even for the most dramatic case of a bias of −300 V. For biases of −450 V and −600 V the count loss is comparable and of a maximum of 15 % after 30 min. A count rate increase after 20 min irradiation is visible for a bias of −600 V at a threshold value of 12.5 keV. Since the measurements have been performed at 600 kHz where count rate limitation play a role, it is currently unclear if the increase in count comes from reduced pile up effects or effects coming from the CdTe.

4 Conclusion

MYTHEN shows good holes and electrons collection capability. The Schottky (Al/CdTe/Pt) diode has proven to have initially good charge collection properties and has a linear energy calibration up to at least 37 keV. It has also displayed a stable behaviour under long term bias when the bias is sufficiently high up to 2 hrs at a room temperature of 24 °C. Under a high flux of $1 \times 10^9$ ph/s/mm$^2$, the sensor appears functional up to 20 min at the same room temperature. This study will be
Acknowledgments

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References


PSIMOD - A generalised system model for investigating the performance of hybrid pixel detectors

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Abstract. Recent advances in hybrid pixel detectors (HPD), motivated by the stringent demands of high-energy-physics experiments, have made a new type of spectroscopically-enabled photon-counting detector feasible. These developments could lead to improved imaging in medical and tomographic applications where detector noise currently imposes limitations. PSIMOD is a generalised system model based on a combination of GEANT4, the TCAD semiconductor simulation package and the SPICE analogue circuit simulation program. It has been developed to reproduce the response of the analogue front end of a pixelated single photon counting detector. With this suite of correlated simulations, it is possible to quickly characterise different system configurations for various detectors.

1. Background
The motivation for implementing modelling techniques lies in the ability to optimize detector development with respect to time and prototyping expenditure. It has been demonstrated that, while the empirical approach is expensive and time consuming, numerical device simulation expedites the design cycle [1]. Adapting the PILATUS [2] hybrid pixel detector system for detection of high-energy photons associated with medical imaging will require replacing the Silicon sensor with a semiconductor material of higher atomic number, such as Cadmium Telluride (CdTe). The ability to model proposed modifications will improve system understanding and expedite the design cycle.

2. Model Configuration
PSIMOD is constructed from three separate simulation packages; GEANT4, TCAD and NGSpice combined with customised glue code. Each program has been designed to accurately simulate a step from probe particle creation to a measured count within the detector, with the information flow from particle to analogue response shown in Figure 1.

Each stage of the simulation chain is modular – programs which provide the same service can be exchanged (GEANT4 can be swapped for G4Beamline [3] for example).
Figure 1: Data flow from particle creation to analogue detector response.

(a) GEANT4 Model

(b) NGSpice Model

Figure 2: Models included in the PSIMOD simulation chain

2.1. GEANT4
GEANT4 \cite{4} is a set of simulation libraries which calculates the motion of a particle through a physical system, taking into account physical processes such as scattering, absorption and particle creation. An example GEANT4 model is shown in Figure 2a.

For PSIMOD, GEANT4 is used to simulate an experimental setup and create an output file describing where incident photons interact with the HPD sensitive area. The HPD active area is described in the GEANT4 simulation as a plane, where each particle impinging on the surface is removed from the simulation immediately after its position (X,Y,Z), energy and particle type is recorded. Currently all recorded particles which are not photons are discarded; an investigation into electrons interacting with the silicon surface is currently being undertaken to extend the model.

2.2. TCAD / DESSIS
Once charge is liberated within the silicon, the approximation of non-interacting particles is no longer appropriate and a different simulation technique is required. Using an FEM (Finite-Element Method) algorithm, DESSIS solves Poisson’s equation on a given set of spatial nodes. Transient solutions can be obtained by allowing the charge elements to evolve a given time-step and solving in an iterative fashion.

A photon interaction in one pixel can result in the splitting of charge into neighbouring pixels. This charge sharing will result in a position dependance on the resultant signal for each pixel, so multiple incident locations on the semiconductor material must be simulated. If it is assumed that the charge is only spread to neighbouring pixels, with symmetry considerations the system reduces to a four pixel system, where the incident charge is deposited in one quadrant of the “center” pixel. The TCAD model for this system is shown in Figure 3. A full simulation using DESSIS is prohibitively slow for every photon interaction to be simulated so a position / energy lookup table is generated prior to running the simulation.

Using a simulation package such as TCAD allows for the calculation of a variety of factors unique to the semiconductor material such as charge sharing, transit time and pulse shapes. It
B.2. PSIMOD - A generalised system model for investigating the performance of hybrid pixel detectors

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(a) Streamtraces which show the trajectory of liberated charge. (b) Detected current from an incident photon.

Figure 3: TCAD/DESSIS Simulation results of a 10 keV photon incident on a PILATUS sensor.

also gives the opportunity to change semiconductor material parameters relatively easily while keeping the rest of the simulation chain intact.

2.3. NGSpice
NGSpice [5] is an open-source implementation of the venerable SPICE simulation package - a powerful tool for analysis of electronic circuits [6]. The description of a circuit is read using the internal NGSpice parser and the system is solved using a set of non-linear differential equations.

Once the induced charge versus time is retrieved from DESSIS, it is included within a circuit as a time varying current source. Transferral of the data from DESSIS to NGSpice is achieved using custom python library construct specifically for PSIMOD which converts the data into a format readable by the NGSpice PWL (Piece-Wise Linear) format. A transient analysis of the system is performed for a predetermined time slice and the output voltage as a function of time of the circuit is written to a binary file.

Figure 2b shows an example analogue front end setup which is implemented in PSIMOD; in this case the current is passed through an amplification stage followed by pulse shaping.

2.4. Python
Although each of the previous simulation packages are powerful tools in their own right, some of the available power is limited by the ability to export data between the programs. It is possible to integrate some of the tool within each other, for example a GEANT4 simulation could in theory be constructed which links to the NGSpice libraries as the source code for both of these packages are freely available. For PSIMOD however each stage was designed as a module which could be swapped or altered easily. This allows an expert in one simulation package to propagate changes through the chain without necessarily being proficient with all the intermediate programs.

A set of Python libraries is used to read in simulation configuration options, run simulations and propagate data from one stage to another. Each stage has a defined input and output datafile format as well as specific simulation options. The Python code also implements much of the digital side of the HPD system, enforcing descriminator levels, re-arm timing and constructing output images.
3. Preliminary Results

Preliminary results of the PSIMOD simulation chain are promising. Initial characterisation of a single-event detector system typically involve discriminator threshold scans in order to calculate the levels required to effectively suppress double counting, fluorescence within the system. Figure 4a shows an example of a threshold scan for 16 keV incident photons at a flux of $1 \times 10^5$ photons per second per pixel. Deviation from the ideal due to the photon pile-up can be seen, with higher gains showing more susceptibility to paralysis than lower gains. Another important characteristic of a discriminating detector is the dead-time of the system which has recently been studied in depth for the PILATUS detector [7]. Figure 4b shows a simulated flux scan versus data measured for the PILATUS HPD system. The PSIMOD Simulation matches the measured drop-off in detector response, though this simulation utilised an analytic form of the analytic front-end and has yet to be repeated with the NGSpice module implemented.

4. Conclusions

PSIMOD has been used to study the effects of proposed modifications on the PILATUS hybrid pixel detector. Using it, the associated dependencies of the various physical processes involved in each stage of data acquisition have been explored. Validation with prototype Silicon sensors provides confidence in the model to now take on the formidable challenges associated with CdTe. Further advances in the simulation package are being investigated, including the introduction of non-ideal components to the analogue circuit simulation and a complete particle interaction model with electrons and heavy-ion charge depositions.

References
Success and failure of dead-time models as applied to hybrid pixel detectors in high-flux applications

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The performance of a single-photon-counting hybrid pixel detector has been investigated at the Australian Synchrotron. Results are compared with the body of accepted analytical models previously validated with other detectors. Detector functionals are valuable for empirical calibration. It is shown that the matching of the detector dead-time with the temporal synchrotron source structure leads to substantial improvements in count rate and linearity of response. Standard implementations are linear up to $0.36 \text{ MHz pixel}^{-1}$; the optimized linearity in this configuration has an extended range up to $0.71 \text{ MHz pixel}^{-1}$; these are further correctable with a transfer function to $1.77 \text{ MHz pixel}^{-1}$. This new approach has wide application both in high-accuracy fundamental experiments and in standard crystallographic X-ray fluorescence and other X-ray measurements. The explicit use of data variance (rather than $\sqrt{N}$ noise) and direct measures of goodness-of-fit ($\chi^2$) are introduced, raising issues not encountered in previous literature for any detector, and suggesting that these inadequacies of models may apply to most detector types. Specifically, parametrization of models with non-physical values can lead to remarkable agreement for a range of count-rate, pulse-frequency and temporal structure. However, especially when the dead-time is near resonant with the temporal structure, limitations of these classical models become apparent. Further, a lack of agreement at extreme count rates was evident.

Keywords: hybrid pixel detector; dead-time; single-photon counting; synchrotron fill pattern.

1. Introduction

Fluorescence X-ray absorption fine structure (XAFS), small-angle X-ray scattering (SAXS) and protein crystallography are important applications of synchrotron radiation that require the position and relative intensity of X-rays to be determined to high accuracy. Widespread use of area detectors for high-throughput crystallography, where the weakest reflection, the strongest reflection and the curve of the diffraction spot profile cover many orders of magnitude of flux and brightness, leads to this being a critical consideration. Further, the temporal structure of recorded spots introduces yet another time dependence to the source. A few attempts on laboratory diffractometers have investigated the absolute calibration and hence linearity of diffracted intensities relative to the straight-through beam (Harada et al., 1970). This necessitates the use of detectors with high radiation tolerance, high dynamic range, low noise performance and a small point spread function. Single-photon-counting pixel array detectors (PADs) such as PILATUS have demonstrated an ability to meet these criteria (Broennimann et al., 2006a; Sobott et al., 2009).

Many other synchrotron applications benefit from these advanced characteristics. Moreover, these advantages serve well in high-flux operation, including measurements of direct-beam or attenuated beam geometries, but also in medium or low-flux operation, including scattering and fluorescence detection from disordered or dilute systems. A range of critical experiments including tests of QED (Pohl et al., 2011; Gillaspy et al., 2010; Chantler et al., 2009a) also depend upon such characteristics of the detector chain. Too often the best measurements are limited by either statistics (detector efficiency and count-rate) or by systematic errors including non-linearities (Chantler & Kimpton, 2009). Hence even modest advances in these areas can lead to dramatic new science. In fact, in several of these fields, an increase in final accuracy by...
2. Analytical models

Two cases of source flux have been discussed and modelled analytically in the literature, that of uniform fill and of bunched fill. While other cases of arbitrary complexity can be modelled using, for example, Monte Carlo methods, in this investigation we explored the exemplars and fundamental ideas via suitable analytic formulations.

2.1. Uniform synchrotron fill

In the case of a uniform fill each bunch contains an almost identical number of electrons and the photon arrival rate can be considered uniform (i.e. Poissonian). A uniform synchrotron fill is an idealization, both experimentally and theoretically, and perhaps might best be modelled with a rotating-anode source.

For a non-paralyzable detector, a signal above a simple discriminator leads to a simple response of the counting system to an incident X-ray rate driving the system, $N_{\text{in}}$.

$$N_{\text{out}} = \frac{N_{\text{in}}}{1 + N_{\text{in}}\tau_s},$$  \hspace{1cm} (1)

where $N_{\text{out}}$ is the observed rate and $\tau_s$ is the dead-time including intrinsic detector and electronic components (Knoll, 1989). Consequently, when the dead-time is constant over all events and events are random in time (Johnson et al., 1966; Reed, 1972; Sharma & Walker, 1992), a relatively simple correction factor can be applied to correct for non-linearity of response.

For a paralyzable detector, each photon restarts the time during which the detector is insensitive to photons and the observed rate is described by (Walko et al., 2011)

$$N_{\text{out}} = N_{\text{in}} \exp(-N_{\text{in}}\tau_s).$$  \hspace{1cm} (2)

Notice that this model results in paralysis, that is, an increasing incident count rate will result in a lower observed count rate. The dead-time is an effective dead-time, as the signal loss may not correspond directly to the dead-time setting on the amplifier but rather is a function of the entire signal processing chain (namely intrinsic and electronic contributions to dead-time).

A third situation may be defined where the paralyzable detector is rejected if the pulses are distorted by pile-up, for example if pulse height analysis (PHA) is performed (Bateman, 2000). The observed count rate can then be described by

$$N_{\text{out}} = N_{\text{in}} \exp(-2N_{\text{in}}\tau_s).$$  \hspace{1cm} (3)

This is similar to (2) but the onset of paralysis is ‘twice as fast’ since the distorted peak does not count as one count but as zero (it is rejected). At high count rates the ability of a discriminator-based system to recover from pile-up and return below threshold is decreased. The losses due to dead-time have a much faster onset because the pulse length must remain undistorted.

2.2. Bunched synchrotron fill

The introduction of single bunches into the beam structure allows the response of the detection system to short bursts of photons arriving at regular intervals to be studied (Honkimäki & Suortti, 2007). If the interval between bunches ($\tau_b$) is greater than the intrinsic dead-time of the detector then the observed count rate is dominated by the bunch spacing. In this case the expected counts from a discriminator-based system, a paralyzable detector or a pile-up rejection system can be described, respectively, by (Bateman, 2000)

$$N_{\text{out}} = \frac{1 - \exp(-N_{\text{in}}\tau_s)}{\tau_b},$$  \hspace{1cm} (4)

$$N_{\text{out}} = N_{\text{in}} \exp(-N_{\text{in}}\tau_s).$$  \hspace{1cm} (5)

This is sometimes called the ‘isolated model’, noting that the shaping dead-time of the detector is irrelevant to the response function. Similarly, if the bunch spacing is reduced to less than the intrinsic dead-time of the detector, i.e. $\tau_s < \tau_b$, the expected counts from a discriminator-based system, a paralyzable detector and a pile-up rejection system can be described, respectively, by

$$N_{\text{out}} = \frac{[1 - \exp(-N_{\text{in}}\tau_s)]/\tau_s}{1 + [1 - \exp(-N_{\text{in}}\tau_s)]/\tau_s},$$  \hspace{1cm} (6)

$$N_{\text{out}} = N_{\text{in}} \exp(-N_{\text{in}}\tau_s(n + 1)).$$  \hspace{1cm} (7)

and

$$N_{\text{out}} = N_{\text{in}} \exp(-N_{\text{in}}\tau_s(2n + 1)).$$  \hspace{1cm} (8)

where $n$ is an integer defined by $n = \text{Int}(\tau_s/\tau_b)$ and describes the discrete nature of the source. For the case where $n = 0$, or $\tau_s < \tau_b$, (6) reduces to (4) and both (7) and (8) reduce to (5).
In addition to investigating the expected benefits to detector linearity from the introduction of a bunched fill, we investigate accepted analytical models as the relation between detector dead-time and bunch spacing approaches resonance.

3. Experiment

3.1. System description

The PILATUS detector system has been described in detail (Broennimann et al., 2006a). Briefly, each PILATUS module comprises 94965 square pixels of side length 172 μm, creating a continuous detector area of 83.78 mm × 33.56 mm. Each pixel comprises the necessary electronics to process and record individual events. Charge liberated in the sensor by incident radiation is transferred to the readout via a microscopic bump-bond (Broennimann et al., 2006b). The signal is subsequently amplified and shaped before discrimination against a pre-determined threshold. If the incident radiation deposits sufficient charge, a local counter is incremented, leading to a complete digital storage of the number of detected events at the pixel level. External bias voltages allow the dead-time of the preamplifier and shaper to be optimized with respect to energy resolution or speed, dictated by the constraints of the experiment. All data presented in this report were acquired with PILATUS; however, results are applicable to any lower-level discriminator-based detector system.

3.2. Australian Synchrotron

The Australian Synchrotron is a third-generation light source (Boldeman & Einfeld, 2004) possessing the key characteristics outlined in Table 1.

Investigations were restricted to fill patterns comprising integer divisions of the revolution time, whilst providing a temporal interval comparable with relevant detector dead-times. Consequently, data were acquired for single-bunch injections with separations of 180 ns and 240 ns. Reference data were also acquired with the standard user fill pattern shown in Fig. 1.

3.3. Measurement

Measurements were undertaken at the Australian Synchrotron Small-Angle X-ray Scattering/Wide-Angle Scattering beamline, utilizing 16 keV radiation. An EPICS (Experimental Physics and Industrial Control System) script was implemented to translate two sets of aluminium attenuators across the field of view of PILATUS. The first set comprised four and the second set 14 attenuators of increasing thickness, resulting in 56 applicable attenuation factors and data points for each shaping time.

Reference images were obtained in the linear region [less than 10 kHz per pixel (Kraft et al., 2009)] of the detector for each attenuator thereby allowing determination of each attenuation factor. The attenuation factor was subsequently used to determine the true incident photon rate from the detected incident photon rate. The accuracy of this low-flux determination is approximately 1–2%, quite adequate for the investigation presented herein, as evident from the data (see §4.1).

Figure 1

The standard user fill, 180 ns bunched and 240 ns bunched patterns as measured with the fill pattern monitor.

Table 1

<table>
<thead>
<tr>
<th>Key parameters of the Australian Synchrotron storage ring</th>
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<tbody>
<tr>
<td>Energy (GeV)</td>
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<tr>
<td>Circumference (m)</td>
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<tr>
<td>Harmonic number</td>
</tr>
<tr>
<td>Revolution time (ns)</td>
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<tr>
<td>Revolution frequency (MHz)</td>
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<tr>
<td>Nominal current (mA)</td>
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In order to avoid counter overflow whilst maintaining adequate statistics, ten sets of 100 ms exposures of the defocused beam were acquired with each attenuator combination. This process was repeated for three shaping times with a standard user fill pattern and for seven shaping times with bunched fill patterns. All data were acquired with a 50% incident energy threshold on PILATUS (Broennimann et al., 2006b) and the response of a single representative pixel is presented in §4. During all acquisitions the electron distribution within the storage ring was observed via a fill pattern monitor (FPM) (Peake et al., 2008). Implemented on the optical diagnostic beamline (Boland et al., 2006), the FPM utilizes a metal–semiconductor–metal (MSM) diode to...
measure incident optical flux and hence infer the stored electron distribution.

4. Analysis

4.1. Model validation for standard or uniform fill pattern

In order to study the relationship between detector response and beam structure, three fill patterns were investigated. Validation was initially performed with the standard user fill, which comprises 600 ns of trapezoidal fill isolated by a 120 ns gap. Data were acquired at shaping times ranging from 125 ns to 383 ns for single buckets separated by 180 ns and 240 ns. The three fill patterns as measured with the FPM are shown in Fig. 1 and the corresponding temporal parameters are presented in Table 2. Summarized in Table 3 are the shaping times used in the measurements. The effective shaping time refers to the effective pulse duration and is derived from previous parameterizations (Kraft et al., 2009).

In probing the models in $\chi^2$, the simplest model was considered first. Results are illustrated for the 180 ns bunched fill in Fig. 2 and fits are based on equation (1), i.e. a uniform fill model without pulse rejection with fixed coefficient $c_s$. Subsequent offset on the $y$-axis for the series of nominal shaping times $C_s$ allowed the model inadequacy to be clearly seen.

The uniform fill model should have been a good qualitative match for the standard user fill, but indeed the model was non-paralyzable and we therefore expected the paralyzable model to match the data. Application of equation (3), i.e. uniform fill with pulse rejection, failed to improve the fits and indicated that this model function was inappropriate. Incidentally, the better of these three uniform fill models was clearly equation (2), i.e. the paralyzable detector without pulse-pileup rejection, and this most nearly approximated the detector type and electronic operation.

Therefore the variance of repeated measurements was used to establish a reasonable and robust input weighting for analysis and to allow the determination of significance in relation to agreement or disagreement with the models previously discussed. Very poor agreement was evident and the corresponding $\chi^2$ values are large. The application of equation (1) to standard user fill data, Fig. 3, also resulted in an extremely poor fit, with reduced $\chi^2$ values for effective shaping times of 125 ns, 200 ns and 384 ns of 68, 33 and 3, respectively. Even in the region where this model should be appropriate, it was clearly and strongly at odds with the data. As far as we are aware, this was the first time that modelling of advanced detector responses and linearity had included explicit variance measures and evaluated goodness of fit using appropriate $\chi^2$ methods. This was crucial as visual inspection could interpret a good fit for lower flux rates even when the model was clearly invalid.

Table 2

<table>
<thead>
<tr>
<th>Fill parameters for the patterns shown in Fig. 1.</th>
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<tbody>
<tr>
<td>User fill</td>
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<tr>
<td>Rise time</td>
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<tr>
<td>Peak</td>
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<tr>
<td>Fall time</td>
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<td>Period</td>
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Table 3

<table>
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<tr>
<th>The seven nominal shaping times investigated.</th>
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<tr>
<td>$C_s(1)$</td>
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<td>-----------------------------------------------</td>
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<tr>
<td>384 ns</td>
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</table>

Figure 2

Measured rate response at each shaping time for 180 ns bunched fill. The corresponding fits are based on a $\chi^2$ minimization of equation (1), i.e. uniform fill model without pulse rejection with fixed coefficient $c_s$. Subsequent offset on the $y$-axis for the series of nominal shaping times $C_s$ allowed the model inadequacy to be clearly seen.

Figure 3

Measured rate response obtained from the standard user fill paralyzable detector with no pulse rejection [equation (2)] with shaping time as a free parameter. The largest shaping time $C_s$ was modelled well while the smallest shaping times were clearly not modelled by the expected non-bunched formula.
To investigate the validity of the shaping time determinations, \( t_b \) was allowed to vary for a fixed bunched spacing. We emphasize that none of these models have more than two parameters, which may be adjusted freely to provide an empirical fit; or constrained such as for a fixed bunch spacing on the assumption that the measurement was at least reflective of an effective bunch spacing within its uncertainty.

For the standard fill pattern, most appropriately represented by a uniform fill model, equation (2), the paralyzable detector without pulse-overlap rejection, the shaping times shifted from 384 ns, 200 ns and 125 ns (predicted/measured) to 355 ns, 201 ns and 136 ns (fitted). Each of these parameters was within one standard deviation uncertainty of the predicted value, and therefore justify both the choice of model and its implementation. However, while \( \chi^2 \) for the longest shaping time was 3, which represented a good fit, the shorter shaping times clearly did not follow this model. Something was missing, either in time structure, detector electronic processing, experimental measurement or uncertainty evaluation, or in some more fundamental understanding of the detector response function at high counting rates. The deviations were systematic and not random, suggesting a causal nature of the discrepancy. It was possible to gain a better empirical fit using a bunched model in some cases, while having two parameters free. However, the use of such a bunched model was unphysical both in model identification and in the parameter values fitted, though it can be quite useful for an empirical understanding of the functional shape at high counting rates.

4.2. Model validation for 240 ns and 180 ns bunched fills: optimized models only

Similarly, for the bunched 240 ns data, with three fills, fitting was undertaken with both shaping time and bunch spacing as free parameters. This resulted in a substantial improvement in the goodness of fit. Fig. 4 represents the best fits for each shaping time, with the bunch spacing and the shaping time as free parameters. The largest four shaping times were best modelled by equation (7) while the shortest three were best modelled by equation (6). This had an unclear physical basis; ideally all should have been best modelled by equation (7). Furthermore, the parameter values obtained were generally unphysical. It followed that this allowed empirical modelling of specific experimental data but the predictive value at this juncture was quite limited. The qualitative understanding of the functional form of the experimental data was nonetheless significantly improved.

Similarly, 240 ns and 180 ns could certainly be correlated in some of the models, yielding a flat \( \chi^2 \) valley and therefore a great difficulty in determining the true minimum. This did not remove the difficulty of the fitted parametrization. A second important point is that the beam optics could in turn shape the bunching further beyond the measured values; while we have no evidence for this effect, it would be reflected in an empirical bunching parameter which was somewhat changed from the measured one, and not as dramatically as was observed.

Some care must be taken in interpreting the results. Arguably the best of these fits was not a good fit, as shown by the \( \chi^2 \) values. The \( \chi^2 \) valley was sometimes very shallow; for example, for the longest shaping time (\( t_s = 384 \) s), \( t_b = 240 \) ns, a value of \( \chi^2 = 30 \) was obtained from equation (7), with parameters \( t_b = 147 \) ns, \( t_s = 237 \) ns, but the same model with fixed \( t_b = 240 \) ns and \( t_s = 144 \) ns yielded the same \( \chi^2 \), as indeed did a model using equation (2) with the single (free) parameter \( t_s = 384 \) ns. In some cases the model form contained parameters which were certainly not independent.

Investigating the \( t_b = 180 \) ns data revealed a similar inconsistency (Fig. 5). No single model fitted the data and...
some conditions were not reasonably fitted by any model, even with all parameters free. Visual inspection alone may look reasonable but all options fail if the reduced \( \chi^2 \) is used as the metric for goodness of fit. Therefore a new model with a more grounded physical basis is required. The bunched fill models, independent of whether the parameters were fixed or free, adequately described bunched data but the choice of models remains inconclusive. The detector was in fact paralyzable (see Fig. 6) so that over longer flux ranges the discrepancies were clear.

As a cautionary note, one should consider the nature of the \( n = \text{Int} (r_s / t_r) \) factor in Figs. 4 and 5. In fitting, the least-squares approach naturally expects continuous variables, so we have modelled the functionals of equations (6) and (7) with \( n = (r_s / t_r) \). The plotted (optimal) fits therefore would be largely summarized or approximated by \( n = 1 \) for the three-bunch settings, \( r_p(1-3) \), and \( n = 0 \) for \( r_p(4-7) \). As the shaping time gets shorter, these models should correctly approach the \( n = 0 \) limit, and the lack of direct physical parameterization of \( t_r \) is not a proper criticism of these models. Ideally, we might anticipate a change-over of \( n \) around \( r_p(3) \) for the three-bunch data and around \( r_p(4) \) for the four-bunch data. While this was not properly observed, this aspect of the bunched models was qualitatively substantiated.

4.3. Model validation post turnover

For a uniform fill pattern the maximum count rate occurs at \( 1 / \tau \), as indicated by equation (1). Increasing the incident flux above this value increases the likelihood of pulse pile-up and reduces the ability of the system to return below threshold. Surpassing the maximum count rate results in a non-monotonic relationship between incident and measured counts, thus introducing ambiguity with respect to the true incident rate. It is therefore important that detector operation is performed below the maximum count rate. However, for complete model comparison, data were acquired well past the turnover point. As seen in Fig. 6, a rate-dependent divergence between the measured and expected counts was clearly evident. There is evidence to suggest that the simple models enumerated in this study, despite being the dominant models of the literature to date, were inadequate to describe fully the operation of these detectors at very high flux.

4.4. Linearity

The complex regions presented correspond to very high flux rates, and indeed empirical fits were found in all cases. However, to examine departure from linearity, a reduced region of interest was defined for Figs. 3, 4 and 5.

Corresponding results are shown in Figs. 7, 8 and 9. Results acquired with the standard user fill pattern indicate that linearity was maintained at the shortest dead-time to approximately 0.36 MHz pixel\(^{-1} \). This value was improved to approximately 0.59 MHz pixel\(^{-1} \) by introducing a 240 ns bunch time gap and to 0.71 MHz pixel\(^{-1} \) by introducing a 180 ns bunch time gap. Improvement was evident across the majority of shaping times, the exception being a shaping time of approximately 260 ns.

Despite the fill pattern producing many photons per bunch, the non-continuous structure of the fill pattern allowed detector efficiency to exceed that indicated by (1). Further, linearity, dead-time and maximum count rate were all improved by a bunched fill pattern. These results demonstrate that the implementation of rate-correction factors to maintain data accuracy outside the linear region of a detector is contingent on an \emph{a priori} knowledge of the fill pattern. Particularly for time-structured fill patterns, any modification to detector dead-time must be coupled to an appropriate applied correction factor.

5. Conclusions and outlook

The rate response of the detector has been compared with expected values from a wide range of accepted models, i.e. the dominant models reported across the literature of electronic detector response functions. Proper \( \chi^2 \) fitting has been introduced and quoted for the first time, and model agreement is specifically characterized by this measure. This has proven that \( \sqrt{N} \) or counting noise was not the dominant cause of variance and hence input experimental uncertainties must be evaluated carefully in all such experiments and investigations.

The functional linearity of the detector chain is excellent, but is critically dependent upon dead-time. The linearity and the maximal count rate measurable with a detector chain is similarly critically dependent upon the matching of dead-time (shaping time) to the storage-ring fill pattern. We have presented all traditional models for dead-time response, and found that empirical fits across wide ranges of flux and time structure can yield good \( \chi^2 \) fits of the data.

While this is valuable for standard synchrotron beamlines including SAXS/WAXS, XAS and XFM applications, it can also find application in traditionally mature fields such as protein crystallography and powder diffraction. This is espe-
cially important as the temporal collection of diffraction spots can combine with many orders of flux and brightness difference for central spots, the weakest reflections collected, and even the profile tails of the weak reflections; and linearity across these dynamic ranges is crucial to structural interpretation. The advances in detector technology and insight can also be dramatic in application to fundamental experiments such as tests of quantum electrodynamics using EBIT where a factor of two reduction in statistical uncertainty or an improvement in linearity can probe new details of the universe (Chantler et al., 2000); and in heavy ion storage rings where temporal structure is also often complex and matching this with the detector chain could be invaluable (Chantler et al., 2007). Of course, recent popular developments with UV and X-ray free-electron lasers have complex and interesting temporal structure as well, arguing for the need for optimal matching of detector chains (Epp et al., 2010). Importantly, there have been recent proposals to join some of these complex sources to investigate fundamental and applied problems in a coordinated manner, for example by merging a synchrotron beamline with an electron-beam ion trap (Chantler et al., 2009b; Simon et al., 2009; Hutton et al., 2009). The resultant spectra will include complexities from the pulse of the fill pattern of the ring, from the usual monochromator optics, but especially from the unique characteristics of the EBIT geometry and source, and even more specifically from the opportunities for temporal pump–probe geometries. The development of these current ideas and their implementation in routine and avant garde experimental configurations will be an important objective.

Future detector fabrication featuring pixel dimensions of 75 μm square (Dinapoli et al., 2010) will afford a factor of five reduction in flux per pixel for a given flux per mm². The smaller pixel size will naturally improve resolution for many imaging applications. If the linearity and maximum count rate limits are similarly scaled, this will be a great opportunity for high linearity in large flux ranges. However, poor agreement between experimental data and theoretical models is evident, in the sense of reliable $\chi^2$ over high-flux regimes and especially in the region where dead-time dominates and the function ceases to be monotonic. Much improved fits are achieved if bunched spacing and shaping times are free parameters within some models, for a range of conditions. Others are not reasonably fitted by any model. This indicates at least one incorrect assumption in (all) the modelling approaches. The model dependence is complex, and the discriminant between model assumptions is sometimes...
weak, especially where the dominant literature models are unsuccessful, and despite useful empirical fits which by eye appear sound. Model validation post turn-over revealed a rate-dependent divergence. We found this an exciting opportunity to understand advanced detector linearity for the first time, for which this investigation was a major step forward. We suspect that there will be multiple causes of the current discrepancies including the difference between an idealized detector response and that of a realistic and complex detector system. A simple suggestion is to investigate Monte Carlo implementations, while correctly implemented, provide no additional insight nor success in this area.

Future work will involve model development to more fully account for experimental results, especially including single photon and Poissonian clustering with temporal fill patterns or bunch cycling times.

A better understanding and control of this matching of temporal structure and detector processing will yield:

(i) Optimized detector linearity (relative accuracy over a discrete range).
(ii) Maximal count rate in high-flux systems (optimized peak value).
(iii) A larger range of usable incoming photon rates.
(iv) Higher efficiency and lower statistical uncertainty in many applications.

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References

Micrometre resolution of a charge integrating microstrip detector with single photon sensitivity

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A synchrotron beam has been used to test the spatial resolution of a single-photon-resolving integrating readout-chip coupled to a 320 μm-thick silicon strip sensor with a dedicated readout system. Charge interpolation methods have yielded a spatial resolution of σx ≈ 1.8 μm for a 20 μm-pitch strip.

Keywords: synchrotron radiation instrumentation; charge integrating; strip detectors.

1. Introduction

The advent of X-ray free-electron lasers (XFELs) such as the European XFEL brings new challenges in detector design. With photon fluxes of the order of thousands or more per detector channel per bunch (bunch length ≳ 100 fs), single-photon-counting detectors are no longer feasible. The Paul Scherrer Institut (PSI) in collaboration with Deutsches Elektronen Synchrotron (DESY) has developed a single-photon-resolving integrating readout chip (GOTTHARD, gain optimizing microstrip system with analog readout) to cope with the high photon rates that will be produced at XFEL (Mozzanica et al., 2010). A charge integrating readout can also be beneficial in synchrotron applications. Photon-counting detectors are rendered ineffective if charge is always shared between multiple strips (Bergamaschi et al., 2008) as is the case for small strip pitches, necessitating the implementation of a charge integrating approach. Additionally, by utilizing analog information the spatial resolution of the system may be improved further via charge interpolation methods (Hubbeling et al., 1991; Brenner et al., 1993; Bergamaschi et al., 2011).

The prototype of the charge integrating system, GOTTHARD, is briefly described in §2. The charge interpolation algorithm is outlined in §3, simulations in §4, and finally the experimental procedure and measured spatial resolution are presented in §5.

2. System description

The GOTTHARD prototype has been designed and integrated with a data acquisition (DAQ) system. The dynamic range and gain switching performance of GOTTHARD are detailed by Mozzanica et al. (2009). The chip is designed in UMC 0.25 μm technology and comprises 100 identical parallel channels. A simplified block diagram of a single channel is shown in Fig. 1. Each channel functions as a low-noise preamplifier with the small feedback capacitor providing the high gain necessary for single-photon resolution. Upon release of the reset switch, charge integration begins on the feedback capacitor such that the output voltage follows \( V_{\text{out}} = -Q_{\text{in}}/C_f \). Dual sample and hold capacitors allow sampling of the output voltage pre- and post-integration time. The difference between the two readouts provides the integrated charge free from any reset noise contribution; this technique is termed correlated double sampling. At the end of each integration time the voltages are serially read out to an external analog-to-digital converter.

Figure 1
A simplified block diagram of the GOTTHARD chip.
research papers

(ADC). To perform the high-resolution measurement, four chips are wire bonded to a 320 μm-thick multi-pitch silicon strip sensor designed by PSI and manufactured by Hamamatsu. The sensor contains pitches ranging from 10 to 25 μm in 5 μm increments, with multiple p+ implant and metalization configurations for each pitch. The DAQ system is based on a field-programmable gate array (FPGA). Analog readout is performed by two 14-bit 80 MHz ADCs. The digital outputs are buffered in the FPGA memory and transferred to an embedded processor, which is controlled by the user PC via a TCP/IP socket interface over 100 Mbit s⁻¹ ethernet. This configuration allows system readout at frame rates up to 300 Hz.

3. Charge interpolation

High-energy physics has shown that by applying non-linear charge interpolation methods it is possible to improve the spatial resolution (Turchetta, 1993; Johnson et al., 2004; Straulino et al., 2006). It is possible to apply a similar principle to an X-ray detector with low noise as was shown by Mozzanica et al. (2010), where a simple analytical approach was used to achieve a spatial resolution of ~3.3 μm r.m.s for a 20 μm pitch. Here, a non-linear interpolation approach, the η algorithm (Turchetta, 1993), is used to optimize the spatial resolution.

3.1. Charge sharing

Incident photons are converted to charge clouds within the sensor and are transported to collection electrodes by the applied electric field. Diffusion and electrostatic repulsion cause broadening of the charge clouds as they drift towards the collection electrode (Lutz, 1999). Charge sharing has been measured to occur in a region of 17 ± 3 μm between the strips, independent of the strip pitch, for a sensor with the same geometry and under equal biasing conditions as used here (Bergamaschi et al., 2008). Therefore, small strip pitches will result in charge always being shared in two or more adjacent strips. As the strip pitch is increased, less charge sharing will occur as the area over which charge is fully collected by a strip increases. Consequently, for large pitches the charge interpolation is not effective over the central strip region and leads to degradation of the spatial resolution. In contrast, very small pitches have a higher inter-strip capacitance Cint, resulting in increased noise, and charge may be shared on more than two strips, degrading the signal-to-noise ratio (SNR) which is defined as the ratio of the mean to the standard deviation of the pulse heights of single photons.

3.2. The η algorithm

The variable η forms the basis of the charge interpolation scheme. If an isolated photon hit is considered, then η is defined as

\[ η = R/(R + L), \]  

where \( R \) and \( L \) are the signals of the right and left channels in the pair, respectively. η may be considered as an average (weighted by the signals \( R \) and \( L \)) of the positions of the adjacent strips located at 0 and 1. The distribution in response to a flat-field illumination is shown in Fig. 2.

Since hits are uniformly distributed over the detector, the position of a hit \( x_0 \) with respect to the left strip may be calculated from

\[ x_0 = p \int_0^\eta \left( \int_0^d (dN/d\eta) d\eta \right) d\eta \]  

where \( dN/d\eta \) gives the differential η distribution and \( p \) is the strip pitch. Equation (2) defines a non-linear algorithm with \( dR/\eta \) given by the integral of the η distribution normalized to the total number of events in the distribution. The positions of the lateral peaks in the distribution shown in Fig. 2 are indicative of the degree of coupling between channels. The width of the η distribution peaks is inversely proportional to the SNR (Turchetta, 1993), from which the standard deviation of the Gaussian noise distribution, or equivalent-noise charge (ENC), is calculated to be 334 ± 8 e⁻ and 370 ± 19 e⁻ for the 25 and 20 μm-pitch channels, respectively. The noise values are in agreement with previously published results using pulse height distribution analysis (Mozzanica et al., 2009).

4. Simulation

For optimization of the reconstruction, algorithm simulations of 20 and 25 μm-pitch sensors are performed as these yielded good results in previous experiments.

Geant4 (Agostinelli et al., 2003), a toolkit for the simulation of particle interaction with matter which is widely used in high-energy and nuclear physics as well as medical applications, is used to generate the initial charge distribution caused by photons impinging on the sensor. Charge transport and charge collection are based on a TCAD (technology computer aided design) layout.
aided design) simulation (Schubert et al., 2010) using finite-element-analysis methods to solve equations responsible for charge transport, generation and recombination. To achieve the required submicrometre spatial resolution over the width of multiple strips, a two-dimensional approach is implemented owing to computational limitations. The simulation is used to study the effects of strip pitch, implant width and sensor thickness and, as a result of this, interstrip capacitance and noise on the performance of the reconstruction algorithm.

A comparison of experimental and simulated \( \eta \) distributions in response to a flat-field illumination is shown in Fig. 3. The lateral peaks of the simulated distribution are nearer to 0 and 1 than those of its experimental counterpart, indicating the simulation underestimates coupling between strips. This is due to the omission of the preamp and more specifically the charge integration occurring on the feedback capacitor in the simulation. For the preamp only the noise is simulated by adding a random noise with a Gaussian distribution to the integrated charge. In the real detector the input of the preamp, and with this the strip, in the sensor has a certain voltage swing during charge integration owing to the limited DC gain of the preamp. This voltage modulation then couples a strip to its neighbours via interstrip capacitances causing a cross-talk between neighbouring strips. In the simulation this cross-talk is lacking and therefore needs to be compensated for via the introduction of a coupling factor, \( K \).

\( K \) is defined as the proportion of charge shared with adjacent strips for the integrated charge per strip for each photon interaction. Simulation shows that a small increase in coupling (see Fig. 3) causes the lateral peaks in the \( \eta \) distribution to shift towards the centre owing to increased charge lost to neighbouring strips. \( K \) ranges from \( \sim 0.05 \) to \( 0.07 \) depending on the strip geometry (pitch, implant size, metalization); this agrees well with the 7% coupling measured for GOTTHARD. The excellent agreement between simulation and experiment provides confidence in the simulation’s predictions, allowing it to be used to explain the origins of features in the experimental data.

To quantify the effectiveness of the reconstruction algorithm a reconstruction error \( \Sigma_R \) is defined for the simulation as \( \Sigma_R = x_i - \mu_i \), where \( x_i \) is the reconstructed position for hit \( i \) and \( \mu_i \) is the corresponding injection position.

Changing interstrip capacitance or noise leads to a significantly different \( \eta \) distribution (see Figs. 3 and 4) which degrades the performance of the \( \eta \) algorithm. In the experiment, significant variation is observed in the noise and gain levels between strips of the same pitch; therefore simulation suggests the \( \eta \) algorithm should be applied independently for every channel pair to optimize the spatial reconstruction. The 20 \( \mu \)m pitch shows greater charge sharing than the 25 \( \mu \)m pitch (see Fig. 5); therefore the reconstruction error for a flat-field illumination is significantly lower for the 20 \( \mu \)m pitch as seen in Fig. 6 (top) for the same noise level. Fig. 6 (bottom) also shows the reconstruction error for photons injected at the strip centre and close to the strip boundary. As expected, the

Figure 3

Top: experimental and simulated \( \eta \) distributions for a 25 \( \mu \)m-pitch strip sensor, normalized to integrated counts. The simulated peaks are closer to 0 and 1 than in the experimental distribution owing to reduced charge sharing as a result of underestimating the strip coupling in the simulation. Bottom: introduction of the coupling factor \( K = 0.06 \) yields agreement within experimental error between experiment and simulation.

Figure 4

Simulated \( \eta \) distribution for ENC = 340 and 390 e\(^-\) which correspond to the minimum and maximum noise values measured for the 20 \( \mu \)m-pitch strips. The Gaussian fits show a broadening of the lateral peaks with increased noise.
reconstruction error is much larger at the strip centre owing to
the much reduced charge sharing. A Gaussian fit to the data
results in a reconstruction error of $1.38 \pm 0.02 \text{ mm}$ at the
strip centre and $0.40 \pm 0.03 \text{ mm}$ close to the strip boundary.

5. Experimental set-up

The following analyses are based on the 20 $\mu$m-pitch sensor
for 15 keV X-rays as this provides the best results. This
presumption is supported by previous experiments as well as
simulation. A simplified diagram of the experimental set-up is
shown in Fig. 8. The sample is mounted on a submicrometre-
precision linear stage, allowing either horizontal or vertical
motion as well as rotation about the beam axis. The stages
have a linear repeatability of 0.4 \text{ mm}. Upstream tungsten slits
permit shaping of the beam impinging on the set-up.

The integration time is selected such that the rate of the
impinging photons per channel is one every few frames,
ensuring isolated hits in each frame, i.e. at least one unoccu-
pied strip on either side of the hit position. The difference
between the pre- and post-integration values is found followed
by a pedestal subtraction and gain correction. Then the
value is calculated for each hit from which the position of the
hit is reconstructed using equation (2). Before any measure-
ments are performed, a flat-field exposure is used to ensure
uniform illumination of all channels from which the relation
between $\eta$ and position is calculated independently for every
strip pair to account for variability between strips. Simulation
(see Fig. 7) indicates that the spread in noise values for 20 $\mu$m-
pitch strips, $334 \pm 8 \text{ e}^-$, amounts to a spatial resolution
variation of approximately 10% across the sensor. The strips
chosen in the analysis are representative of the average noise
values and can therefore be said to yield the average spatial
resolution for the sensor.

5.1. Spatial resolution measurement

The spatial resolution of a system may be determined by
measuring its response to a point source; this is termed the
point-spread function (PSF), which is experimentally attained
here and validated via simulation. A 2 $\text{mm}$ tungsten slit is
placed in front of the sensor parallel to the strips and scanned
across several strips in 1 $\text{mm}$ increments with $3 \times 10^4$ frames
acquired at each step. Comparing motor position to recon-
structed position, as shown in Fig. 9, yields the error on the
reconstructed position, which is a convolution of the PSF and
tungsten slit width. A larger reconstruction error is observed

Figure 5
Simulated $\eta$ distribution of the 20 and 25 $\mu$m pitches for a coupling of $K = 0.06$ and ENC = 390 $\text{e}^-$. Compared with the 25 $\mu$m pitch, the peaks of the 20 $\mu$m-pitch $\eta$ distribution exhibit a significant shift towards the centre of the $\eta$
distribution and a higher plateau at the centre, indicating a greater degree of charge sharing.

Figure 6
Top: reconstruction error (difference between reconstructed and injection position) for a simulated flat-field illumination of the 20 and 25 $\mu$m pitches for an ENC of 340 $\text{e}^-$. The smaller pitch shows a smaller reconstruction error. Bottom: reconstruction error distributions for the 20 $\mu$m-pitch strip for injection positions 0 $\mu$m (centred on the left strip) and 8 $\mu$m (close to the strip border) shown for an ENC of 340 $\text{e}^-$. The differences between the two distributions are due to little charge sharing at injection point 0 $\mu$m. Gaussian fits give a reconstruction error of $1.38 \pm 0.04 \text{ mm}$ at the strip centre and $0.40 \pm 0.03 \text{ mm}$ close to the strip boundary.
at the strip centres [as predicted by simulations in Fig. 6 (bottom)] owing to noise having greater impact in this region of the distribution.

The asymmetry observed in the PSF in Fig. 9 is due to an asymmetry in the scan region. From Fig. 9 the PSF is calculated to be approximately Gaussian with $\sigma_x \approx 1.8 \pm 0.1 \text{ mm}$; this forms a conservative estimate of the resolution as the contribution from the beam width and motor resolution are not subtracted. The experimental PSF is compared with a simulation of a 2 mm square-profile beam scanned over several strips and is calculated via the same reconstruction procedure as outlined here with the exception of adjusting for gain variation and DC offset, as these are not present in the simulated data owing to the exclusion of all electronics. Simulation of a 2 mm-wide square beam scanned over adjacent strips is shown for comparison in Fig. 9; the resulting PSF is a Gaussian distribution with $\sigma_x \approx 1.3 \pm 0.1 \text{ mm}$ for an ENC of 340 e$^-$. The difference between simulation and measurement stems from effects which are not taken into account in the simulation such as the beam divergence and the uncertainty in the alignment of the slit parallel to the strips. The uncertainty of the alignment is estimated to be $1\degree$, with a beam height of 100 mm; this already causes an uncertainty of 1.7 mm. The resolution measurement is therefore currently limited by our ability to align the slit parallel to the strips. Fig. 7 demonstrates a lower limit for the reconstruction error of $\sigma_x \approx 0.8 \text{ mm}$ for the 20 mm-pitch strip. With an optimized set-up, in particular in terms of slit size, a resolution of the order 1 mm should be achievable.

5.2. Periodic structures

The applicability of the reconstruction algorithm is tested with scans of various microstructures. The structures are formed via $\sim$3 mm-thick gold on 300 mm silicon and include a series of lines of varying thickness, where the pitch is equal to twice the strip width. The 2 mm slit is placed a few millimetres in front of the sensor, as shown in Fig. 8, whilst the gold line sample is kept statically in front of the slit with the sample lines orientated parallel to the strips. $2 \times 10^5$ frames are acquired with an integration time of 1 ms. Even though the fabrication of narrower lines on the test sample is in principle

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**Figure 7**

$\sigma_x$ of the simulated PSF as a function of ENC for the 20 and 25 mm-pitch strips with a coupling of $K = 0.06$ at 15 keV. As expected, the spatial resolution degrades with noise.

**Figure 8**

Simplified diagram (not to scale) indicating the positions of the strip sensor, the 2 mm slit, the sample and the direction of the incoming parallel beam for all microstructure scans. The sample is scanned vertically or horizontally depending on the measurement.

**Figure 9**

Top: motor position versus reconstructed position giving an indication of the reconstruction error. A 20 mm segment spanning two strips, with 0 mm and 20 mm corresponding to adjacent strip centres, is shown. Blurring of the line is a maximum at the strip centres. Bottom: quantifying the reconstruction error. This is approximately equivalent to the detector PSF for which the $\sigma_x$ of the experimental profile is measured to be 1.8 mm. The simulated PSF for a 2 mm-wide square beam with ENC = 340 e$^-$ and a coupling of $K = 0.06$ is also shown.
possible (Gorelick et al., 2010), line widths of 10 μm or greater were chosen for testing owing to their adequate quality and ease of alignment. As seen in Fig. 10, the measured contrast of the 10 μm lines is 52 ± 8%, from which the thickness of the gold layer is estimated to be 2.2 ± 0.2 μm, which is compatible with the sample character. The line width is measured to be 10.4 ± 0.9 μm and therefore demonstrates the possibility of reconstructing structures smaller than the strip pitch. The tungsten slit scan confirms that smaller structures down to sub-2 μm are resolvable, prompting a future attempt at producing and measuring the smaller pitch gold structures.

5.3. Complex structure test

The experimental procedure is as described in the previous section (§5.2); however, the sample is now scanned vertically, and 2 × 10^7 frames per 1 μm motor step are acquired. The charge interpolation algorithm is applied as for the tungsten slit scan. The reconstructed image seen in Fig. 11 is on an angle and contains a modulation owing to misalignment of the sample with respect to the strips and distortions in the slit, respectively.

The line width of the letters is ~7 μm as seen in the scanning-electron-microscope image in Fig. 11. Averaged cross sections of the vertical components of the letters H and T are used to determine the FWHM of the lines to be 8.6 ± 1.3 μm.

6. Conclusions and outlook

It has been demonstrated that the charge integrating chip GOTTHARD in combination with a 20 μm-pitch strip sensor is capable of resolving sub-2 μm structures using a non-linear charge interpolation approach. The simulation of the resolution shows that the measurement is limited by the experimental set-up and not the detector. The reconstruction of 50 μm-high letters demonstrates the high-resolution imaging capability of the charge integration approach over single-photon-counting systems at low count rates. If the noise is reduced to 100 e−, as is the case for a pixel detector, then from Fig. 7 it is predicted that submicrometre spatial resolution may be achieved.

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References

research papers


Defect Structures in Diamond Composite Coated Cemented Tungsten Carbide Substrates

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Keywords: Diamond properties and applications, PCD coated carbide, Wear, Residual stress

Abstract. Variability in the abrasive wear of PCD coatings on cemented WC substrates has been investigated. Six samples of PCD coated carbides were tested in a wear testing rig. The PCD coated element was used to turn an industry standard vitrified bonded corundum grinding wheel. The wear rate was measured as the weight loss of the cutting element per cubic metre of grinding wheel machined during the test. Two grades of cutting elements were observed. One grade had wear rates between 6 and 7.3 g/m$^3$ but of the three poor quality samples, only one valid test was made realising wear rate of ~7,800 g/m$^3$. The microstructures of the samples were studied using SEM, X-ray imaging, neutron diffraction and XRD. SEM images revealed differences in the volume percentage of diamonds in the two grades and the XRD scans highlighted the variable distribution of the diamond phase in the coating. Estimates of the residual stresses in a good and poor quality samples indicated significantly higher compressive stresses in the good quality versus poor quality coating. These results have revealed two extremes in the wear rates of these PCD coated carbides. It is suggested that the difference in diamond content between the two grades is not sufficient to account for the 3 orders-of-magnitude difference in the observed wear rates. However, the presence of intrusive veins of carbide material in the coatings, especially around the curved cutting tip, suggested that the macroscopic defects observed in the x-ray and SEM images were the major cause of the high wear rates in the poor quality sample.

Introduction

Diamond based tooling has been used extensively for many years in the mining and manufacturing industries \cite{1,2,3,4}. Konstanty \cite{5} devised a classification based on the manufacturing processes used to produce these tools. Apart from tools utilising loose diamond powders and single crystal diamonds, most diamond tools consist of polycrystalline diamond materials in either composite or single phase format. In the case of diamond coatings on cemented WC-Co, the coating has traditionally consisted of a diamond-cobalt composite with the diamond concentration usually greater than 85 volume percent. Such diamond composite coatings are not rated as thermally stable and are limited to machining operations in which the temperature is unlikely to rise above 800°C for any length of time. Thermal stability is achieved by (a) single phase diamond coatings produced by CVD, (b) etching out the cobalt binder or (c) using a catalytically inactive binder such as SiC \cite{5-8}.

The specific area of interest in this study is the variation in abrasive wear rates of diamond composite coatings on WC substrates as a function of composition and structure at the micro and macro scale.
Experimental

The samples used in this study consisted of diamond composite (DC), coated cemented WC-Co. These samples were purchased commercially but no specific information was supplied as to the manufacturing process, coating thickness and the exact composition of the diamond coatings except they were designated as consisting of polycrystalline diamond (PCD) coatings moulded onto specifically shaped WC-Co substrate – they were manufactured under high pressure, high temperature conditions (HPHT) within the diamond stability field at approximately 1550°C and 5.5 GPa. Each sample was assessed for its wear rate using the severe abrasive wear testing procedure previously described in detail by Li and Boland [6]. In summary the wear testing conditions were as follows:

- counter wear surface consisted of a vitrified corundum wheel of industrial standard;
- speed of wear test, 30 m/s;
- a set “depth-of-cut” of 0.3 mm as set for each traverse of the 50 mm wide wheel and a nominal 100 cuts were used, although for poor quality tools, this number was reduced;
- loading on the tool was measured using a load cell mounted on the sample holder;
- abrasive wear rate was calculated as the weight loss of the tool per cubic metre of wheel cut.

The worn surfaces were examined in an SEM equipped with an X-ray energy dispersive detector. Further studies of these surfaces were made using an X-ray diffraction apparatus (GADDS) with an X-ray spot size of ~600 microns. The top coated section of selected samples were sectioned longitudinally using electrical discharge machining (EDM) and the cut-surfaces were polished to assist in additional characterisation studies of the coatings. An X-ray imaging system was used to detect macrostructural defects in the coatings of these sectioned samples while further microstructural examination of the coatings was made in an electron probe microanalytical system equipped with a cathodoluminescence (CL) detector system. Finally, measurements of the residual stresses in the coatings were made using neutron diffraction.

Results

The results of the wear testing on a suite of coated samples are shown in Table 1. A clear distinction can be made between good quality, wear-resistant coatings and poor quality samples. Samples from batches 1 and 2 had wear rates below 10 gm$^{-3}$ while samples in batch 3, purported to be PCD coatings, showed extremely high wear rates.

<table>
<thead>
<tr>
<th>Sample ID</th>
<th>Number of cuts</th>
<th>Wear distance (m)</th>
<th>Wear rate (g/m$^3$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-2</td>
<td>100</td>
<td>3394</td>
<td>7.1</td>
</tr>
<tr>
<td>2-3</td>
<td>100</td>
<td>4176</td>
<td>7.3</td>
</tr>
<tr>
<td>2-4</td>
<td>100</td>
<td>3399</td>
<td>6.0</td>
</tr>
<tr>
<td>3-1</td>
<td>10</td>
<td>379</td>
<td>14589</td>
</tr>
<tr>
<td>3-4</td>
<td>4</td>
<td>152</td>
<td>7816</td>
</tr>
<tr>
<td>3-8</td>
<td>2</td>
<td>76</td>
<td>7823</td>
</tr>
</tbody>
</table>

1: Weight loss of test sample per cubic meter of grinding wheel removed in the test.

Fig. 1 shows the wear pattern in a good (2-4) and a poor quality sample (3-1). Clearly the poor quality sample 3-1 had worn through to the underlying WC substrate. In cases where the substrate is revealed, the test was classified as invalid and for the samples in batch 3 the test had to be limited to two cuts.
SEM studies of the worn surface showed immediately that the poor quality samples had a lower than expected diamond concentration – Fig. 2. In this backscattered electron image, the dark phase is the diamond while the matrix is predominantly WC with some Co also present. Unlike diamond impregnated metal matrix composites (MMC) in which the diamond grains are frequently plucked out of the MMC, there was no evidence of this wear mechanism in these worn surfaces.

**Fig. 1.** Wear patterns in diamond composite coated cutting elements. (a) top view before, (b) top view after wear test and (c) perspective of sample 2-4 after 100 cuts. (d) top view before, (e) top view after wear test and (f) perspective of sample 3-1 after only 10 cuts – WC diameter, ~20 mm.

**Fig. 2.** SEM backscattered electron images from the worn surfaces of samples 2-4 (left) and 3-1(right).

Samples 2-4 and 3-1 were sectioned using EDM and examined using (a) X-ray imaging of the coated segment (Fig. 3) and (b) GADDS-XRD system for phase identification – Fig. 4.
In sample 2-4, there was an artefact produced during the EDM operation in which a section of the coating spalled off – this is evident in Fig. 3 (a). Nevertheless, the distinctive image of the coating showing the macroscopic defects at the substrate-coating interface is clearly revealed – see also Fig. 5 below for a higher magnification of a specific macro defect. Unexpectedly, the coating in 3-8 did not show up in the X-ray image - Fig. 3 (b). This observation substantiated the SEM studies in which the mean diamond concentration in batch 3 samples was ~46 volume percent resulting in an insufficient density contrast between the substrate and the coating.

The XRD studies revealed that samples in batches 1 and 2 had significant amounts of ZrC. This result is shown in Fig. 4, while samples in batch 3 consisted of diamond and WC as the major constituent phases.

Cathodoluminescence (CL) was also used to reveal the phase distribution in the diamond composite coating. Cross correlation of X-ray images with SEM and CL images revealed the nature of the macroscopic defects in the DC coatings. This was clearly demonstrated in Fig. 5 in which a crack initiated at some stage in the HPHT sintering process resulted in the intrusion of the substrate material into the overlying diamond composite coating. This sample was from a separate batch of diamond coated WC substrates but the wear rate was extremely low, being ~ 4 gm^-3.

Preliminary neutron diffraction studies have been made on the coatings in samples 1-2 and 3-4. For 1-2 the residual stress in the diamond phase was calculated as -910 +/- 31 MPa. For 3-4, the residual stress in the diamond was -354 +/- 37 MPa and for the WC phase, -406 +/- 64 MPa. It was not possible to obtain unambiguous measurements from the minor ZrC phase in 1-2 although it was clearly identified in the XRD traces.

**Discussion**

The results of this study have revealed that the abrasive wear rates of diamond composite coatings on WC-Co substrates are strongly dependent on the quality of the composite. Confronted by the marked differences in wear performance of these three batches of coated cutting elements, it was essential to investigate the underlying microstructures and compositions of the coatings. These observations have highlighted the major differences between the samples. From SEM studies, it was clearly shown that the good quality coatings from batches 1 and 2 contained much higher diamond concentration but in addition, the composition of the matrix or binder component was very different. ZrC was the dominant second phase in the good quality composite. Although a carbide former [9], ZrC is more likely to be an aid to sintering rather than a product of reactive sintering/bonding as occurs in the thermally stable diamond composites in which Si is added.
Significantly, none of the worn surfaces showed evidence of diamond grain being plucked from the matrix indicating strong bonding between the diamond and composite matrix. The dominant influence on the wear resistance of the coatings appeared to be the diamond concentration. Further investigations of the overall stability of the diamond phase are currently underway using Raman spectroscopy and detailed micro-XRD studies.

Sample 2-4 GADDS XRD trace original surface

Sample 3-1 GADDS XRD trace original surface

Fig. 4. XRD traces showing all major peaks for samples 2-4 and 3-1.
Summary
The abrasive wear behaviour of commercially produced PCD-coated, cemented WC-Co tools has been shown to depend on both phase composition of the coating and the presence of macroscopic defects in the coatings. Samples with ZrC – presumed to have been added as a sintering aid - and a high concentration of diamonds had the best wear resistance. Samples with a low diamond concentration and no evidence of the sintering aid ZrC had wear rates up to three orders of magnitude greater than the good quality samples.

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B.5. Defect Structures in Diamond Composite Coated Cemented Tungsten Carbide Substrates

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Defect Structures in Diamond Composite Coated Cemented Tungsten Carbide Substrates
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Wear Resistance and Microstructural Study of Diamond Coated WC Tools

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Keywords: PCD, WC, abrasive wear, electron microprobe, cathodoluminescence, mapping, hyperspectral, diamond centre, x-ray imaging, tomographic reconstruction, photon-counting, pixel detector, Pilatus, neutron diffraction, residual stress, Raman spectroscopy

Abstract. Diamond composite materials are classified as superhard and exhibit exceptional abrasive resistance. Cemented tungsten carbide tools with a thick coating of diamond composite material (PCD) are finding increased usage in materials cutting operations in manufacturing, mining, minerals, gas and petroleum exploration and civil construction industries. Two major advantages derived from these coated tools are: (a) increased wear resistance and hence increased life-span of these tools and (b) their proven ability to handle “difficult-to-machine” materials as well as high-strength, extremely abrasive materials such as quartz-rich rocks, granites and basalts. In this research, the variability of the wear resistance of PCD coated tungsten carbide is correlated with microstructural variations. A detailed study of the microstructure and distribution of phases was performed using SEM, cathodoluminescence (CL) imaging, direct x-ray imaging, Raman spectroscopy as well as residual stress measurements using neutron diffraction.

Introduction
Diamond coated tools are being used with increasing frequency across a wide range of industries covering exploration, mining and manufacturing industries [1,2]. In the manufacturing industries, the coatings are usually of the order of 10-50 microns thick and in the main are deposited by the CVD (chemical vapor deposition) process [3]. In mining and civil construction industries PCD (polycrystalline diamond composite) cutting elements are commonly used [4,5]. These coatings are usually much thicker being in the range of 0.1-1 mm. The outstanding advantage of such coated cutting elements in rock cutting tools is the increased life of the tools because of the superior wear resistance of diamond composites compared with the traditional cemented carbide cutting tools [6].

Previous microstructural and wear studies of diamond composite cutting elements have been directed to thermally stable diamond composites (TSDC) [7,8]. This study examined the abrasive wear rates of PCD coated WC cutting elements and correlates their wear behaviour with micro- and macrostructural features in the PCD coatings.

Experimental Procedures
Samples consisting of a thick coating (0.5-1.0 mm) of PCD, specially moulded onto cemented WC substrates were purchased from a commercial supplier. The wear testing was performed on CSIRO’s...
testing rig described elsewhere [7]. As-worn samples were examined in an SEM and then residual
stress measurements were made using neutron diffraction. For this study two grades of samples were
selected: one good and the other poor quality. Cathodoluminescence images were observed on
polished sections in an electron probe microanalytical (EPMA) system while the x-ray attenuated
images were recorded by a single photon counting pixel detector (PILATUS) using a Hamamatsu
micro-focus source (8 microns, 70 keV & 80 μA).

Results

Abrasive wear and microstructures of PCD coated tools. Details of the microstructures and wear
rates are given in Figs 1 & 2 and Table 1.

Fig. 1 Good quality PCD coated sample: top view of worn surface (a) optical (sample diam. 20 mm)
and (b) backscattered SEM image of worn PCD surface.

Fig. 2 Top view of poor quality PCD; (a) optical image showing wear extended through to the WC
substrate (sample dia. 20 mm) and (b) backscattered SEM image of worn PCD surface.

Table 1 Wear rates and microstructural details of PCD coating on WC substrate

<table>
<thead>
<tr>
<th>Sample ID</th>
<th>Wear rate of PCD coating, [g/m³]</th>
<th>Average diamond grain size, [microns]</th>
<th>Volume percentage diamond</th>
</tr>
</thead>
<tbody>
<tr>
<td>Good quality</td>
<td>6</td>
<td>15.1</td>
<td>57</td>
</tr>
<tr>
<td>Poor quality</td>
<td>7,800</td>
<td>13.6</td>
<td>39</td>
</tr>
</tbody>
</table>
The attenuated x-ray image and the combined SEM-CL images of a polished PCD coated sample are shown in Figs 3 & 4.

**Fig. 3** Attenuated x-ray image of coating on WC substrate showing macrocracks within the PCD coating - see Fig. 4 for the microstructures within the selected area.

**Fig. 4** (a) Backscattered electron image and (b) combined x-ray and CL image composed of W – blue, Co – green (both images derived from the wavelength dispersive spectrometers) and diamond – red (derived from the CL spectrum across the wavelength band: 250 – 980 nm).

**Stress measurements.** Neutron diffraction measurements were made at ANSTO research reactor using the stress scanner Kowari [9] to determine the von Mises stress \((\sigma_{\text{M}} = |\sigma_{22} - \sigma_{11}|)\) (equivalent tensile stress) in the two 20 mm dia. samples (PCD coatings in the samples were 1.2 mm and 0.9 mm respectively). Our experimental data (Fig. 5) suggest that the poor quality sample had stresses significantly lower than the good quality sample.

**Spectroscopic analysis.** Initial measurements of Raman spectra, using 633 nm laser excitation, were inconclusive due to excessive fluorescence signal that masked the characteristic peaks of the diamond (1332 cm\(^{-1}\)) or any other carbon phase such as graphite (D and G peaks [10]). The fluorescence effects can be reduced by using IR laser excitation and this research is being planned.
Fig. 5 von Mises stress, $\sigma_{22} - \sigma_{11}$, for both diamond and WC phases for the good and poor quality samples. Experimental results were determined with accuracies of 160 MPa in WC and 60 MPa in diamond phase – the frame of reference is shown for the coated samples.

Discussion

The difference in abrasive wear behaviour of the two 20 mm dia. PCD coated tools is clearly related to the nature of the defect structures at both the micro- and macro-scale. Residual stress measurements on the larger samples indicate stress relaxation has occurred in the poor quality sample, most likely resulting from micro and macro cracking. This explanation is supported by the x-ray images showing distributed cracking within the PCD coating. Minor differences in diamond grain size and volume percentages (Table 1) are unlikely to account for the vast difference in the wear rates. Other microstructural features such as the multiple defect zones in diamond need to be studied using high resolution CL imaging on EPMA and micro-XRD to resolve the differences in wear behaviour of these PCD coatings.

References

B.6. Wear Resistance and Microstructural Study of Diamond Coated WC Tools

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