Development of a 25 micron pixel detector for phase-contrast imaging

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Abstract

High spatial resolution, high-efficiency, low-noise and energy discrimination are detector features needed for many X-ray applications, in particular the ones related to imaging. In this thesis two charge integrating silicon detectors are investigated. Charge-integrating detectors can exceed many limits of single photon counting detectors. The pixel size can be much smaller, since less electronics is needed per pixel in the read-out chip. With charge integrating detectors it is possible to detect the energy of the absorbed photon, which is proportional to the generated charge in the sensor. Additionally, compared to photon counting detectors, where the charge sharing between pixels limits the minimal pixel size, the spatial resolution can be increased by investigating the charge sharing between neighboring pixels using the analog information, thus allowing even more spatial information than given by the pixel size and position.

In this thesis two charge integrating detectors developed at the Swiss Light Source are investigated. A one-dimensional strip detector with a strip pitch of 25 $\mu$m and a two-dimensional pixelated hybrid detector with a pixel size of $25 \times 25 \mu m^2$. These detectors are optimized and are most efficient in the energy region from 3 $keV$ up to 30 $keV$. The pixelated detector was characterized, and a method to exploit the charge sharing effect to gain additional position information was developed. The developed method was tested in experiments with an X-ray tube and also at the synchrotron. One of the key findings answered with these experiments was the measurement of the spatial resolution of the detector together with the assessment of the position interpolation methods. A position resolution on the micrometer level was achieved.

The main motivation for the development of the interpolation method is its application to grating based phase contrast measurements. With the grating interferometer a fringe, that is a Talbot self-image of the phase grating, is recorded. Since the sample changes the fringe pattern, it is possible to deduce the phase change introduced by the sample. The phase change encodes information about the material properties of the sample and is especially interesting for weakly absorbing materials common in biological and medical imaging. The main limitation of this setup is the resolution of the detector. To resolve the fringes with detectors that have not enough spatial resolution, an analyzer absorption grating is stepped in front of the detector. This stepping procedure requires high mechanical stability of the setup, increases the acquisition time and the deposited dose in the sample, and thus prevents medical applications. In this thesis I show experimentally, that small pitch charge-integrating detectors are capable of resolving the fringes without the help of an analyzer grating. This is possible by using the developed method to investigate the charge sharing between neighboring pixels. With the experiments I successfully demonstrated that the analyzer grating is not needed, which could be a major step towards the medical applicability of grating based phase contrast measurements.
Zusammenfassung


In Rahmen dieser Doktorarbeit wurden zwei am Swiss Light Source neu entwickelte ladungsintegrierende Detektorsysteme getestet. Zum Einen ein Streifendetektor mit 25 \( \mu m \) Streifenbreite, zum Anderen ein Pixeldetektor mit einer Pixelgröße von \( 25 \times 25 \mu m^2 \). Diese Detektoren haben eine hohe Effizienz für harte Röntgenstrahlen im Bereich von 3 \( keV \) bis 30 \( keV \). In dieser Doktorarbeit wurde die spektralen Eigenschaften des Pixeldetektors charakterisiert, sowie eine Methode entwickelt welche die zusätzlich verfügbare Information über die Photonenenergie und die Ladungssteilung zwischen Pixeln auswertet und ein hochaufgelöstes Bild inklusiv Photonenenergie liefert. Die Methode wurde ausführlich mit einer Röntgenröhre sowie am Synchrotron getestet. Dabei wurde auch die Auflösung des Detektorsystems im Zusammenhang mit der erwähnten Methode evaluiert. Eine Positionsauflösung im Mikrometerbereich wurde erreicht.

Die Hauptmotivation für die erhöhte Positionsauflösung ist das Aufnehmen von Phasenkontrastinformation mit Hilfe eines Gitterinterferometers. Bei diesem Interferometer wird mithilfe des Talbot-Effekts ein Interferenzmuster, welches ein Abbild des Phasengitters ist, aufgezeichnet. Die Probe verändert das Interferenzmuster, wobei unter Berücksichtigung der Änderung die Phasenverschiebung durch die Probe bestimmt werden kann. Die Phasenverschiebung erlaubt insbesondere für biologische und medizinische Proben Rückschlüsse auf die Materialeigenschaften. Der limitierende Faktor beim Gitterinterferometer ist die Auflösung des Detektors, da die Verschiebung des Interferenzmusters maximal wenige Mikrometer beträgt, und der Abstand der Interferenzspitzen typischerweise ebenfalls wenige Mikrometer beträgt. Um das Interferenzmuster trotz limitierter Auflösung zu detektieren, wird heutzutage meist ein Absorptionsgitter vor dem Detektor schrittweise durchgeschoben. Diese Prozedur verlangt eine hohe mechanische Stabilität des Aufbaus, verlängert die Erfassungszeit und erhöht die Dosis, da typischerweise die Hälfte der Röntgenstrahlen die Probe zwar durchdringen, aber nicht detektiert werden. Mit dieser Arbeit wurde experimentell gezeigt, dass die Auflösung der ladungsintegrierenden Detektoren, unter Anwendung der Methode, welche die Ladungssteilung zwischen Pixeln auswertet, hoch genug ist, und das Interferenzmuster direkt aufgelöst werden kann. Dies vereinfacht den Aufbau des Git-
ter interferometers, da das Absorptionsgitter nicht mehr benötigt wird, und bietet die Perspektive gitterbasierte Phasenkontrastmessungen medizinisch zu nutzen.
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Chapter 1

Introduction

1.1 Previous work and motivation

Wilhelm Röntgen detected X-rays on the evening of 8 November 1895. He discovered, that running
a high-voltage discharge tube let a barium platinocyanide sheet fluorescence, even tough the tube
was enclosed in a cardboard box. He concluded, that the tube must emit some unknown form of
radiation and named the radiation X-rays. Later on, Röntgen discovered that X-rays also expose
photographic plates and he created the famous first X-ray images of his wife’s hand. For his
discovery, he was awarded with the very first Nobel prize in physics in 1901.

Until the 1920s, cold cathode or Crookes X-ray tubes were used. These first generation X-
ray tubes generated the electrons, needed to create X-rays, by ionizing residual gas in the tube.
One major disadvantage of this design was, that the glass of the tube slowly absorbed the gas
while exposed to X-rays. Therefore, the pressure inside the tube decreased and a higher voltage
between the anode and cathode was required to ionize the gas. With this higher voltage, the tube
generated a harder X-ray spectrum and stopped working eventually when most of the residual gas
was absorbed.

In 1913, William Coolidge developed the hot cathode tube, the second generation X-ray tubes,
. By producing the electrons with a hot tungsten filament as cathode, these tubes were no longer
dependent on residual gas in the tube. The filament is heated by an electric current. These
Coolidge tubes are still used today, although the design was improved. For high output tubes the
rotating anode was developed. While the anode is spinning, the surface area, were the electrons
are absorbed and the X-rays are produced, is increased. This reduces the heat load per area and
allows a higher electron and therefore X-ray flux.

For experiments where a small focal spot size is required (such as, e.g. micro-imaging) micro-
focus X-ray tubes are available. The small spot size is possible by having a narrow focused electron
beam hitting the anode. Since the mechanical imbalance of the rotating anode would increase the
spot size, the electron beam density is limited, thus allowing these tubes to run only on little
power. With metal-jet-anode micro-focus X-ray tubes, the output power could be increased by
replacing the solid anode by a liquid metal jet. This allows to cool down the anode material while
it is not in the beam, without having the disadvantage of the rotating anode.

The first observation of synchrotron radiation from a cyclotron was at General Electric in
New York in the year 1947. It was not until 1961, when the National Institute of Standards
and Technology (NIST) modified its 180 MeV electron synchrotron to extract the radiation via
a tangent section in the vacuum system. In 1963 united states politics decided to build a new
high-energy accelerator near Chicago, Illinois. It was later named Fermi National Accelerator Laboratory. In 1964 the trend towards higher energy synchrotrons took a big leap with the commissioning of the 6 GeV Deutsches Elektronen Synchrotron (DESY) in Hamburg, Germany. It was used for high-energy physics and for producing synchrotron radiation. Nowadays, there are many third generation synchrotrons in all parts of the world. The planning of the Swiss Light Source (SLS) at the Paul Scherrer Institute in Switzerland, where some experimental data for this work was acquired, started in 1991. The project was approved by 1997 and first light was seen in the year 2000 [1]. The 2.4 GeV storage ring has a circumference of 288 m and seventeen operational beamlines [2]. Main focus of research at the SLS are material science, biology and chemistry.

Since there is a great variety of conducted X-ray experiments, the requirements for X-ray detectors are also very broad. Therefore, the development of detection methods, starting with simple photographic plates, went in many different directions. The principle of the Geiger-Müller tube was proposed by Hans Geiger in 1908 and was developed further by Walther Müller and Geiger in 1928. In the 1970s newly developed semiconductors allowed to convert X-rays directly into electrical current. In 1980 Fuji presented a first prototype of images plates, that are nowadays replacing the photographic plates and film in the medical field almost entirely. Results of the first silicon strip detectors for high energy physics were published by the CERN and PISA group in 1980 [3][4]. First hybrid pixel detectors were successfully used in the WA97 experiment at CERN in 1994 [5]. In 1998 Medipix-1, a photon counting detector with 64 × 64 pixels, dedicated to X-ray detection was tested and characterized [6].

The development of photon counting hybrid detectors for X-rays went on, and they are nowadays well established at synchrotrons. A few popular devices in use are, e.g. PILATUS [7], EIGER [8], Medipix3RX [9] and IMXPAD [10]. However, due to the pulsed structure of the beam, they are unsuitable at X-ray free-electron lasers (XFELs). In the last few years, this boosted the development of charge integrating hybrid detectors like CSPAD [11], GOTTHARD [12], AGIPD [13], DSSC [14], LPD [15] and JUNGFRAU [16]. These detectors deliver the same data quality as photon counting detectors [17], while overcoming some of their disadvantages, e.g. the minimum detectable energy, the saturation at high count rates and the limits on the pixel size due to charge sharing [18, 19].

The majority of medical X-ray imaging techniques still rely on the attenuation contrast, in which the differences of the radiation absorption properties of the object reveals the internal structure. The absorption property of materials is dependent on the density of the material. Biological and medical sample usually consist of low density material, that have similar low absorption. In comparison, phase-contrast imaging [20] provides an alternative approach for distinguishing structures by detecting distortions of a wavefront as it propagates through the sample. This distortions originate from changes in the refractive index of the sample. For low density samples, such as biological and medical samples, the change of the phase is much stronger, than the absorption. Therefore, recording the phase contrast gives more image information at the same dose than an absorption contrast image. A key advantage of phase contrast imaging is, that the electron density distribution of the sample can be characterized without the need for radiation absorption [21].

Zernike first developed the principle for phase contrast imaging with visible light in 1942 [22]. The transfer of Zernikes discovery to the X-ray range took until 1965, when Bonse and Hart proposed a first X-ray crystal interferometer, made from a large and highly perfect single crystal [23]. The crystal only accepted a narrow energy band and was therefore only suitable for synchrotron applications. Another major step towards simplification of phase contrast imaging was the propagation based imaging technique developed at ESRF (European Synchrotron Radiation Facility)
in 1995 [24]. In 2002 Christian David and colleagues adapted the Talbot grating Interferometer, that was previously successfully demonstrated in atom interferometry [25], for hard X-rays at a synchrotron beamline [26]. It is not until the introduction of the Talbot-Lau Grating Interferometer (GI) [27] and later coded aperture [28], that sensing phase and small-angle scattering contrasts simultaneously and effectively [29] on conventional X-ray tubes became possible, and thus a major step to use the method for clinical applications was made. To evaluate the potentials of this technique, extensive studies have been carried out, spanning from radiography [30] to computer tomography [31]. Promising applications have been demonstrated for mammography [32, 33], human hand imaging [34, 35] and lung imaging [36].

Despite of the promising results, implementing a grating interferometer suitable for clinical practice remains a challenge [37]. One complexity for the system design is the employment of the analyzer grating (commonly known as $G_2$). The success of GI relies on resolving very subtle distortions in the interference fringe caused by the refraction (usually in sub micro-radians) of X-ray photons. The system sensitivity (minimal resolvable refraction angle) is mostly given by the pitch of the interference fringe [38], which is in the range of a few micrometers. Directly resolving the fringe of such small pitch is beyond the capability of most detectors. The use of $G_2$ with a pitch matching the period of the interference fringe, successfully decouples the system sensitivity and the pixel size by adopting a mechanical scanning protocol known as phase stepping [39].

However, this phase stepping procedure is generally time-consuming and demands high mechanical stability for good image quality. Single shot (in contrast to phase stepping) phase contrast imaging methods have been proposed, using larger pitch gratings [40]. Nevertheless these methods compromise the sensitivity and spatial resolution of the system. Another major problem of using $G_2$ is the dose issue. The presence of $G_2$ dumps half of the photons that pass through the sample due to the 50% spatial duty-cycle. Further, X-ray tubes, even those installed in modern medical imaging devices, have a limited power and are operated at their limits. A $G_2$ in the beam path requires an increase in scanning time, sometimes incompatible with experimental or medical acquisition protocols.

To resolve the fringe produced by the grating interferometer directly, a high spatial resolution (in the order of microns) is required. With hybrid pixel detectors, with pixel sizes in the range of tens of microns, this is only possible with single photon based spatial resolution interpolation. There has been a variety of studies in the field of high-energy physics and X-ray detection, to enhance the spatial resolution of particle tracks and photon hits. In 1993 investigation on the spatial resolution properties of silicon strip detectors to enhance particle tracking in high-energy physics experiments started at CERN [41, 42]. Other studies [43] investigated the charge sharing effect in silicon and gallium arsenide sensors with a Medipix1 chip [44] and photons up to 35 keV. At lower photon energies (up to ∼ 8 keV) charge-coupled devices (CCDs) under direct illumination of X-rays were investigated for high-resolution large area detectors with single photon resolution [45, 46]. For up to 17.4 keV sub-pixel resolution algorithms for fully depleted pn-junction CCDs with a pixel size of 75 × 75 $\mu$m$^2$ were developed [47]. Centroiding algorithms also play an essential role for position reconstruction of signals from micro-channel plates (MCP) [48, 49]. Previous studies of the SLS Detector Group [50, 51, 52] showed, that it is possible to exploit the charge sharing effects to achieve sub-pixel position resolution in silicon hybrid strip and pixel detectors for X-rays [53].
1.2 Scientific aim

The main scientific aim of this work is to evaluate the feasibility of using hybrid detectors for phase sensitive X-ray imaging methods, like the Talbot Laue interferometer without $G_2$. This involves, tests and characterizations of newly developed small pitch hybrid detectors in lab environments and at different beamlines. Further on, this involves adaption of the well known interferometers, by simplifying the setup to make it more mechanically stable and better suitable for real applications. Additionally, development of algorithms to analyze the output of the detector to extract the phase information is necessary. The following paragraphs will explain these parts in more detail.

The detector group at Swiss Light Source (SLS) developed two type of detectors suitable for the use in a $G_2$-less grating interferometer. GOTTHARD is a one dimensional hybrid strip detector with a channel pitch of 25 $\mu m$. MÖNCH is a pixelated hybrid detector with a sensitive area of $0.4 \times 0.4cm^2$ and a pixel pitch of $25 \times 25$ $\mu m^2$. Initial experiments were performed with GOTTHARD. Once MÖNCH was available in an early development stage, further experiments were conducted exclusively with MÖNCH. To perform experiments with these detectors a read-out system and firmware for the system had to be developed.

For phase contrast imaging two types of algorithms need to be developed. First, the position interpolation algorithms responsible for reconstructing the position of each photon with highest possible resolution. Second, phase retrieval algorithms that are insensitive to variable distortions originating from the position interpolation algorithms. This work also involves testing and evaluating different existing and newly developed algorithms.

Currently used grating interferometer consist of a source, an optional source grating, the sample, a phase grating, an analyzer grating and the detector. It is difficult to place this various mechanical components in a stable fashion along the beam. Most critical is the stability of the phase and analyzer grating with respect to the detector. To simplify this part, the analyzer grating is omitted and the detector must have the ability to detect the fringe, which is produced by the phase grating, without the analyzer grating. This can generally be achieved by high resolution detectors, but current high resolution detectors generally have low efficiency and need long acquisition times. The previously mentioned detectors (GOTTHARD and MÖNCH) have the ability to have high position resolution while preserving a high photon sensitivity, and are therefore suitable to perform the detection of the fringes without an analyzer grating. In biological or medical applications, the high efficiency of GOTTHARD and MÖNCH potentially allows to reduce the dose compared to the measurement with the analyzer grating.
Chapter 2

X-ray imaging concepts

This chapter covers the concept of imaging with hard X-rays. First, the different X-ray sources are discussed, namely X-ray tubes and synchrotrons, then some concepts of X-ray interaction with matter are reviewed. In the last part, the requirements of X-ray detectors for different applications are specified and a non-exhaustive list of detector technologies is presented.

2.1 X-ray production

2.1.1 X-ray tube

An X-ray tube (XRT) contains a cathode and an anode in a vacuum tube. The cathode is a heated filament that releases electrons into the vacuum. The high-voltage between the cathode and anode accelerates the electrons towards the anode. The anode has a target surface that is usually tilted towards the exit window of the XRT. The material of the target surface is commonly molybdenum, chromium, copper, silver or tungsten. When the accelerated electrons hit the target, X-rays are produced by bremsstrahlung. Then they cause fluorescence and the If the electron energy is high enough to remove inner electrons of the target atom a characteristic (fluorescent) XRT line is emitted (see figure 2.1).

To have a spot-like X-ray source the absorption surface on the anode is preferable small. To still have a high power output, the electron beam density should be high. The absorption of this high density electron beam generates a substantial amount of heat that must be dissipated. Therefore, modern XRT have a rotating anode, where most of the target is not in the beam and has sufficient time to cool down.

Depending on the target material the resulting X-ray spectrum looks different. The spectrum produced by an XRT is comparable to a broad bremsstrahlung spectrum with the superimposed fluorescence lines of the target material (see figure 2.1). The applied high-voltage between anode and cathode limits the acceleration of the electrons, and therefore the maximum photon energy of the resulting X-rays. The current flowing from the anode to the cathode (usually some mA) does not alter the shape of the spectrum, but linearly scales the photon beam flux. The photon beam flux has also an approximately square relationship to the applied high-voltage [54].

2.1.2 Synchrotron

Synchrotron radiation is emitted if a charged particle, that travels close to the speed of light (i.e. relativistic), is accelerated. In a synchrotron, electrons are accelerated to relativistic speeds
by a linear accelerator and a booster ring. After that, they are injected into a storage ring. To follow the ring curvature, they are accelerated radial towards the ring center by bending magnets. During this acceleration the electron beam emits synchrotron radiation in tangent direction by bremsstrahlung. The spectrum of this synchrotron radiation is continuous and starts at terahertz radiation up to hard x-ray radiation (see figure 2.2).

In addition to the bending magnets, insertion devices are used to produce synchrotron radiation in modern third generation synchrotrons. An insertion device is an array of dipole magnets with alternating polarity. While traversing the insertion device the electron beam follows an undulated trajectory and emits synchrotron radiation. There are two types of insertion devices. In the wiggler the electron beam undulates with high amplitude and the resulting X-ray beam has high energetic photons. The intensity of the X-ray beam is proportional to the electron beam. In the undulator the electron beam undulates with lower amplitude and therefore the radiation spectrum is limited to lower X-ray energies, but the radiation from the different dipoles interfere positively with each other. The intensity of the resulting X-ray beam has a squared dependency from the number of dipole magnets. This increases the brilliance of the resulting synchrotron radiation.

Smaller synchrotron, like the SLS, have 10 to 20 bending magnets and undulators with an associated beamline. The beamlines are optimized for different experiments, and therefore the optics of the beamlines differ. Usually they have a monochromator that filters the broad synchrotron spectrum to one narrow band spectrum with an energy resolution down to $\delta E/E = 10^{-4}$. Most modern beamlines rely on insertion devices placed in the straight sections of the storage ring. Tomcat, the imaging beamline at the Swiss Light Source, where most experiments of this work are carried out, is installed after a super-bend magnet.

2.2 Interaction of X-rays with matter

Understanding the interaction of X-rays with matter is essential to exploit X-rays for a variety of applications, such as crystallography, high resolution microscopy, X-ray material science and biological and medical imaging. X-rays, or more general all light, can be simultaneously described by waves or particle. To explain the interaction with matter we focus on the particle properties
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Figure 2.2: Spectrum of synchrotron radiation of a bending magnet. Electron energy: 2.4 GeV. Ring Current: 400 mA. Magnetic Field: 2.9 T \[56].

of X-rays in this chapter. For a brief description of the wave model by focusing on refraction and reflection see section 5.1.

Photons travel at the speed of light have no mass and are electrically neutral. They do not continuously interact with matter, but rather penetrate the matter unaffected up to some distance and deposit their energy at one point. Photons produced by X-ray tubes and synchrotrons interact mostly with the electrons of the matter (see figure 2.3). For an initial photon beam with a flux of \( I_0 \) the attenuated flux after the material can be calculated by:

\[
I = I_0 e^{-\mu \rho z},
\]

(2.1)

where \( \mu \) is the mass absorption coefficient of the material penetrated, \( \rho \) is the material density and \( z \) is the traveled distance through the material \[57\]. \( \mu_l = \mu \rho \) is also denoted linear absorption coefficient. The mass absorption coefficient is related to the total atomic cross section \( \sigma_{tot} \):

\[
\mu = \frac{N_A}{A} \sigma_{tot},
\]

(2.2)

where \( N_A = 6.022 \times 10^{23} \text{ mol}^{-1} \) is Avogadro’s number and \( A \) is the atomic weight \[57\].

In the energy range of interest for this thesis, there are three distinct types of interactions between photons and electrons: photoelectric effect, Thomson scattering and Compton scattering. Each of these types contributes to the linear absorption coefficient:

\[
\mu_l = \mu_{pe} + \mu_{coh} + \mu_{incoh},
\]

(2.3)

where \( \mu_{pe} \) is the contribution of the photon effect, \( \mu_{coh} \) from the Thomson effect and \( \mu_{incoh} \) originates from the Compton. The cross-sections of several processes involved in the interaction of X-rays with matter are shown in figure 2.3, for the example of carbon. Note that, in the energy range of X-ray tubes and synchrotrons, only the three mentioned processes contribute significantly to the total cross-section. These processes are now described in more detail.
Figure 2.3: Cross-sections of carbon for photoelectric effect ($\tau$), Compton scattering ($\sigma_{\text{coh}}$), total measured cross-section ($\sigma_{\text{tot, experiment}}$) and cross-sections from other effects. The step in $\tau$ at 284.2 eV is the K-edge of carbon. The unit barn is equal to $10^{-24} \text{cm}^2$. From [57] with data from [58].

2.2.1 Photoelectric effect

The photoelectric effect describes a process, where the photon is absorbed and the energy of the photon is transferred to an electron. Conservation of momentum dictates, that the recoil momentum of the released electron has to be absorbed. Therefore, a complete absorption of the photon energy is only possible with the bound electrons of an atom [59]. The photon ejects the electron only, if its energy exceeds the binding energy of the electron on its shell. Electrons in outer shells are therefore rejected at lower photon energies than inner bound electrons.

The probability of absorption of the photon is highest for electrons closer to the nucleus [59]. If the photon ejects a core electron, an electron from an outer shell may fall into the vacancy. This process results in an energy surplus, that can either be released by emitting a single fluorescence X-ray or by transferring the energy to an outer shell electron that is then ejected (see figure 2.4). The ejected electron is called Auger electron. The ratio between the two competing processes is called fluorescence yield. For higher $Z$ materials ($Z > 31$) the fluorescence emittance dominates [60].

2.2.2 Thomson scattering

Thomson scattering describes an elastic process, where an electron is sinusoidally accelerated by the incoming electromagnetic field. During the acceleration the electron itself emits light of the same energy [61]. If we assume that the incoming field is linearly polarized the emission coefficient at an angle $\chi$ is:

$$\epsilon = \frac{\pi \sigma_{\text{coh}}}{2} I \cos^2(\chi),$$ (2.4)
2.2. INTERACTION OF X-RAYS WITH MATTER

Figure 2.4: Photoelectric effect. The incident photon is absorbed and the energy is transferred to a bound electron. (a) The electron is ejected from the shell. (b) An electron from an outer shell may fall in the vacancy. (c) This will release energy either by emitting an X-ray photon or by emitting an Auger electron from an outer shell.

where $\sigma_{coh}$ is the Thomson cross section of the electron and $I$ is the incident flux. Therefore, the intensity of the re-emitted radiation has an angular dependency (see figure 2.5). Orthogonal to the incoming beam there is no light re-emitted, since the projected oscillation amplitude of the electron is zero. On the other side the photon emission parallel to the incoming beam is highest.

The Thomson cross section can be derived under the assumption that the incoming and outgoing photons have the same energy:

$$\sigma_{coh} = \frac{8\pi}{3} r_e^2$$

(2.5)

where $r_e$ is the classical electron radius.

2.2.3 Compton scattering

Experimental results from Compton in 1922 showed that photons scattered from material can have less energy than the incident photons [62]. This inelastic process could not be explained by Thomson scattering. Later experiments have shown that the Thomson formula is only valid for non-relativistic energies, where $h\nu << m_e c^2$.

Towards higher energies one has to consider the quantum nature of light which permits the description of the Compton effect. Compton scattering describes the effect, when a photon is scattered by an electron and loses part of its energy. The loss of energy increases with a higher scattering angle $\theta$. The energy lost by the photon is transferred to the recoil electron which is emitted in a angle $\phi$ to the incoming photon. The energy transferred to the recoil electron can have a maximum energy defining the so-called Compton edge. The angles of the recoil electron and the
2.2.4 Absorption process for the used energy range

At the Swiss Light Source the energy range is up to 40 keV. In this thesis X-ray energies in the range from 8 keV up to 20 keV were used. The dominant process for the presented measurements is therefore the photoelectric effect.

2.3 X-ray detection

Since the early days of the discovery of X-rays, research was focusing on the development of X-ray detection methods. For imaging purposes photographic film served long as a good detection method and it was only at a later state that image plate detectors, scintillation detectors and most recently semiconductor detectors were used in that domain. In other X-ray research areas other detectors with more suitable properties for the specific experiments were developed. The following section explains some detection technologies and later some figures of merit of X-ray detectors are discussed.

2.3.1 X-ray detector technologies

There are a variety of different X-ray detection methods, each has different properties and is therefore suitable for different tasks. This section is a brief overview of common detectors.

Film based systems are still in use for medical imaging and other X-ray applications. They provide a high spatial resolution, that is only limited by the thickness of the sensitive layer. The main disadvantage of this system is the low dynamic range. The sensitive layer is composed of a gelatin containing silver compound and is deposited on a flexible support layer. The silver
compound grains have a diameter of around 1 \( \mu m \) \cite{59}. When the silver compound grains are exposed to photons, one or more electrons are released from the atom. When the electrons slow down they are eventually caught at trapping centers within the grains. If the film is developed the conversion of the illuminated grains in to black metallic silver is amplified \cite{59}.

**Image plates** consist of a flexible substrate with small photo-stimulable phosphor crystal on top. The crystals are covered with a protective layer. The phosphor, while exposed to X-rays, is capable of storing a fraction of the X-ray energy. The stored energy is emitted later by photo-stimulated luminescence, if the phosphor is stimulated with visible light. The emitted light is proportional to the stored X-ray energy and its frequency is reasonable separated from the stimulation light, such that the stimulation light can be filtered away while reading back the stored intensity \cite{63}. Compared to X-ray film the dynamic range is a factor \( 10^5 \) higher and the read-out speed of 5 to 10 \( \mu s \) per pixel is also higher. Image Plate detectors are commonly used in medical applications and have been used in protein crystallography at synchrotrons \cite{63}.

**Gas detectors** consist of a closed containment where incident X-rays ionize a gas. The incoming photons creates ions and free electrons proportional to their energy. An applied electric field across the containment collects the charged particles at the anode and cathode. Gas detectors have not a high spatial resolution.

In the case of ionization chambers the electric field is strong enough, such that the ions and electrons are separated before they recombine. This will generate an electric current across the chamber that can be measured and is proportional to the dose the gas is exposed to.

For proportional counters the geometry of the anode is such that the electric field is stronger towards the anode. This causes the drifting electrons to ionize further gas molecules, creating an avalanche effect. This avalanche effect creates a spike in the current that is proportional to the energy of the absorbed photons. Therefore, counting the photons and detecting the photon energy is possible by analyzing the spikes.

Geiger-Müller counter use a very strong electric field so that UV-photons are created if a photon is absorbed. The UV-photons ionize new gas molecules and eventually all the gas around the anode is ionized. This generates a very strong signal at the cost of a high detector dead-time after a particle is detected.

**Scintillation detectors** consist of a special material that converts the X-rays into visible light photons. The visible light is then transported via light guides or lenses to photomultiplier tubes, photo-transistors or CCDs. One major advantage of this concept is, that conventional optics can be used to magnify the image. Common scintillation materials are NaI(Tl), CsI(Na) or GdOS(Tb) \cite{57, 64}. The scintillation material and thickness influences the properties in terms of detection efficiency, temporal and spatial resolution. They are commonly used at imaging synchrotron beamlines and also for X-ray tube imaging.

**CCD detectors** are in wide use for digital cameras in consumer products and are therefore available in many different varieties. For imaging experiments with energies lower than 1 \( keV \), direct exposure of a back-thinned CCD detectors yields good results. At higher energies, a scintillation material converts the X-rays into visible light, which is then detected by the CCD. CCD detectors are available with high pixel count and small pixel sizes down-to to 4 \( \mu m \). Compared to
other detection methods, CCDs have a low frame rate and a limited dynamic range, due to the serial read-out and the full well capacity.

**Hybrid pixel detectors** consist of a sensor connected to a read-out electronics. The sensor material can be a variety of semiconductors, whereas the read-out electronics is an application specific integrated circuit (ASIC) on a silicon substrate. For strip detectors the electronics is commonly wire-bonded to the sensor, whereas for the pixel detectors bump-bonding is used. The hybrid assembly allows for separate processing and optimization of the two parts and also increases flexibility in the choice of the sensor material.

Each sensor segment (i.e. pixel or strip) of the sensor is electrically connected to a read-out channel. In the case of pixel detector the connection is realized with a small bump (indium or solder), that also provides mechanical connectivity.

There are two major read-out designs in use nowadays. The single photon counting detectors (SPCs) have a digital counter in each channel, that is incremented if a photon above a certain energy level is detected. The read-out is fully digital and very simple, but the count rate of these detectors is limited. A new concept was developed for higher count-rate requirements, that are usually encountered at experiments with free electron lasers. The charge integrating detector (CID) does no longer discriminate the photons by incrementing a counter in the channel on the ASIC, but integrates the amplified charge produced by the photon absorption. Compared to SPCs, this concept has the advantage, that there is no dead-time after a photon is detected. This is a requirement for free electron lasers, since the photons arrive simultaneously (i.e. in femto seconds).

Currently the most commonly used sensor material is silicon. The conversion coefficient of silicon is $\sim 3.6 \text{ eV per electron hole pair}$. Hybrid pixel detectors have a high dynamic range, count-rate capability and quantum efficiency. On the other side, the segmentation is limited due to the interconnection between read-out chip and sensor.

For an overview of the semiconductor hybrid detectors developed at the Swiss Light Source see [18]. The detectors used in this thesis, namely GOTTHARD and MÖNCH are described in depth in section 3.5 and section 3.6.

### 2.3.2 X-ray detector requirements

**Signal-to-Noise ratio (SNR)** Photonic noise is present in every measurement and is due to the fluctuations of photon arrival rates in the space and time domain. It obeys the Poisson statistics. The amount of absorbed photons in a time and space unit will result in a statistical distribution with $N$ as mean and $\sqrt{N}$ as standard deviation. Therefore the minimum signal-to-noise ratio of a detector system is given by:

$$\text{SNR} = \frac{N}{\sqrt{N}} = \sqrt{N}. \quad (2.7)$$

Note that increasing the amount of absorbed photons by rising the pixel size, exposure time or photon flux will result in a higher SNR. Depending on the detector system the SNR can be reduced by subsequent processing steps. For example the read-out electronics can add additional noise and will therefore reduce the SNR.

**Quantum efficiency** is the ratio between input to the sensor versus output from the sensor:

$$\text{QE} = \frac{I}{I_0}, \quad (2.8)$$
2.3. X-RAY DETECTION

where \( I_0 \) is the amount of incoming photons and \( I \) is the amount of absorbed photons by the sensor. In the case of a semiconductor detector this is the ratio between impinging photon flux versus electron-hole pairs collected at the output of the sensor. The quantum efficiency depends on the thickness and the type of the sensor material (see e.g. figure 3.2).

The detective quantum efficiency (DQE) defines the ratio between output SNR to input SNR:

\[
\text{DQE} = \frac{\text{SNR}_{\text{in}}}{\text{SNR}_{\text{out}}}. \tag{2.9}
\]

The DQE can be different to the QE if the absorption process introduces additional noise (see Fano noise or the modulation transfer function for example).

Spectral resolution The Spectral Resolution of a detector describes the capability to distinguish energy levels of detected photons. It is expressed in eV either as full width at half maximum (FWHM) value or as the standard deviation of the detected spectrum of a monochromatic beam. There are several noise contributions to the spectral resolution.

In an analog read-out the spectral resolution is directly related to the read-out noise of the detector. Therefore noise contributions from the read-out electronics have a significant impact to the spectral resolution of the detector. Read-out noise is measured in equivalent noise charge (ENC) with number of electrons as unit. It defines the root mean squared noise of the output as a signal change variation at the input. The ENC is estimated by measuring the noise after the read-out electronics and then back-calibrate it to the input by estimating the amplification of the read-out electronics. By considering the conversion coefficient of the sensor material the equivalent noise charge can be converted into the spectral resolution with unit eV.

Electron-hole pairs are produced, if a photon is absorbed by a semiconductor. This process is a statistical process, with a mean amount of pairs produced per absorption. The variance of this process is called the Fano noise and is one limitation of the energy resolution of the detector. The Fano factor \( F_f \) is a material property and is introduced as an adjustment factor to relate the variance of the electron-hole pair production to the Poisson theory predicted variance. Therefore, if \( F_f = 1 \) the electron-hole pair production is a purely Poissonion process with a variance equal to the square-root of the mean pair production. If \( F_f = 0 \) the amount of produced electron-hole pairs has no event-to-event variance and is constant for all absorption events. For a silicon semiconductor \( F_f \) is 0.115 and for CdTe and GaAs \( F_f = 0.10 \) [65]. For systems with a scintillator \( F_f \) is higher and usually around 1 [66]. Figure 2.6 shows a simulation of the Fano noise contribution, if one photon is detected. Depending on the conversion efficiency and the Fano factor of the sensor material the impact changes. In the energy range and with the sensor material used in this thesis the contribution of the Fano noise to the spectral resolution are negligible compared to other noise contributions.

Temporal resolution describes the ability of the detector to distinguish photons, that are closely separated in time. The sensor of a system has a collection time, i.e. the time needed for collecting the signal by the anode in a gas or a semiconductor detector, or a decay time, i.e. the time delay introduced by a scintillator while converting X-ray photons to visible photons. This physical property of the sensor has usually a value in the order of nanoseconds (for gas or semiconductor detectors) and up to milliseconds for scintillation based systems.

Count rate capability is limited by the frame-rate, the dynamic range and the pixel size of the detector and is measured in photons per area and time, i.e. in hits \( \text{mm}^{-2}\text{s}^{-1} \). Modern single
Figure 2.6: The noise contribution to the spectral resolution from the Fano noise, if one photon is absorbed. 4 different sensor materials are considered.

Photon counting detectors for synchrotrons have count rates up to $1.8 \times 10^{10}$ hits mm$^{-2}$s$^{-1}$ [67], while count rates of $10^9$ hits mm$^{-2}$s$^{-1}$ are common in medical imaging [68]. Newly developed charge integrating detectors for free electron laser facilities reach even higher count rates.

**Spatial resolution** The spatial resolution can be determined as position resolution for single photons or for two photons. In photon science usually the second one is used, i.e. the spatial resolution is an indication, for how close in space two photons can be, so that they are still distinguishable by the detector. It is measured by the point-spread function (PSF) in the space domain or the modulation transfer function (MTF) in the frequency domain. The MTF shows the maximum contrast a detector can reproduce at a given spatial frequency. The frequency is represented in line-pairs per mm. Figure 2.7 (a) shows two example PSFs. One is from a detector system with a Gaussian response (e.g. a scintillator system) and one from a system with a box response, i.e. where the pixel size is the limiting factor. Systems with strips or pixelated system can be limited by the pixel size and a box response is possible. Note that both PSF are normalized, i.e. the total detected intensity is 1 in both cases. Also note that the standard deviation of both PSFs is the same ($\sigma = 7.22 \, \mu m$), since the standard deviation of a continuous uniform distribution is given by:

$$\sigma = \sqrt{\frac{1}{12} p^2}, \quad (2.10)$$

where $p = 25 \, \mu m$ is the pixel pitch or the width of the uniform distribution. Figure 2.7 (b) shows the same detector response as the MTF. At low spatial frequency, the response is similar and drops continuously. At higher frequencies the pixel-size limited system has aliasing effects, once the Nyquist frequency of 40 lp/mm is reached.

To measure the PSF, the detector is exposed to a point-beam with significant smaller diameter than the expected resolution of the detector system. After the acquisition the point-beam will be convoluted with the PSF of the detector. If one can assume that the point-beam has no contribution to the PSF (since it is much smaller than the PSF), the resulting image corresponds to the PSF of the detector.
2.3. X-RAY DETECTION

Figure 2.7: (a) shows the PSF of a system with a Gaussian response and an expected response from a pixelated detector. (b) MTF of the two systems. (c) and (d) show a simulated acquisition of a grating with variable spatial frequency. The resulting image is a convolution of the sample and the Gaussian PSF (c) or the pixel PSF (d) of the detector.

It is also possible to directly measure the MTF, by acquiring an image of a grating with various spatial frequencies. By measuring the intensity difference between absorbing and transparent regions, i.e. the contrast, it is possible to populate an MTF plot. Figure 2.7 (c) and (d) show a simulated acquisition of a grating with variable spatial frequency, starting from 1 lp/mm (line-pair per millimeter) up to 60 lp/mm. The sample grating is convoluted with the Gaussian PSF with a σ of 7.22 μm or a box PSF with a pitch of 25 μm, respectively (both PSFs shown in Figure 2.7 (a)). By correlating the contrast of the recorded sample grating and the known spatial frequency, the MTF plot can be visualized (see Figure 2.7 (b)). At low frequencies (below 20 lp/mm), the difference in the response between the two detector systems is insignificant. At higher frequencies, the detected contrast is diminished for both. However, at 40 lp/mm the contrast of the pixel-size limited system reaches zero and recovers at higher frequencies. This is due to to aliasing effects. Chapter 4 explains a position interpolation method that is capable to overcome the resolution limitation for strip and pixel detectors due to segmentation as mentioned previously (see equa-
This is possible under certain conditions and assumptions. First, the charge of each detected photon is detected by multiple adjacent pixels. This effect is explained in section 3.3. Second, the impinging photon flux is tuned, such that in each acquisition less than one photon is detected per pixel cluster. And third, the range of charge generated by a photon is known, since a rough estimation of the beam spectrum is available. Under these conditions and by looking at each photon absorption individually, it is possible to determine the photon absorption position with a finer resolution than the pixel pitch would allow.

Since the previously mentioned position interpolation method analyzes the signal height of each pixel of a cluster, it is limited by similar factors like the spectral resolution. For example, the electronic noise has a significant impact in the final position resolution.

**Dynamic range** quantifies the ratio between the smallest detectable signal and the maximum signal per exposure. For CCDs the full-well capacity (FWC) specifies the maximum charge that can be stored per pixel without overflow to neighboring pixels. In digital CCDs the range of the analog-digital converter (ADC) is tuned to match the FWC. For example a CCD camera with 16 bit dynamic range can have a signal difference of a factor of $2^{16} = 65536$ between the smallest and the highest detected signals in an image. For photon counting detectors the dynamic range is limited by the depth (in bits) of the counter per pixel or strip. Common counter depths are ranging from 4 bits for fast acquisition up to 24 bits [67]. Single photon counting detectors like Eiger have a negligible read-out time allowing to sum images off-line. Therefore, these detectors can have a dynamic range only limited by the exposure time. For charge integrating detectors, one possibility to quantify the dynamic range is in charge equivalents of $12\text{ keV}$ photons. Depending on the intended experimental environment, the dynamic range of a charge integrating detector can start at $\sim 1$ $12\text{ keV}$-photon up to $10^5$ $12\text{ keV}$-photons for free electron laser experiments.

**Radiation tolerance** X-ray radiation has destructive effects on all detector parts present in the X-ray beam. 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. Surface damage includes changes in the covering dielectrics and interface region and manifests as an increase in leakage current [69]. With hybrid pixel detectors the electronics is behind the sensor and receives a fraction of the radiation, since the sensor has a finite absorption efficiency. X-ray radiation has destructive effects on the oxide layer in the field-effect transistor (FET) and diminish its performance. As an example, figure 2.8 shows the noise performance of a pixelated silicon hybrid detector after different amount of radiation. [70] presents an exhaustive measurement of the radiation tolerance of a hybrid silicon pixel detectors.
Figure 2.8: Electronic noise performance of a JUNGFRAU detector after different amount of dose for three different acquisition lengths. After a certain dose, the radiation has a significant impact on the noise performance of the detector. Note that also the pixel to pixel variation (indicated by the error bar) increases after a certain dose [70].
Chapter 3

X-ray hybrid semiconductor detectors

In the first part of this chapter a basic overview on hybrid detectors is given. In section 3.2 the relevant properties of silicon semiconductors are presented, and also how the detection of X-ray photons with silicon sensors works. In section 3.3 the charge sharing between pixels is explained, and initial thoughts how charge sharing can be modeled are shown. Section 3.4 shows the two major methods for amplifying and detecting the charge generated in the sensor. In section 3.5 and section 3.6 the two hybrid detectors used for all experiments in this thesis are presented. In the last section a quick overview of the data acquisition system is shown.

3.1 Hybrid detectors

The detectors used in this thesis are so-called hybrid detectors. Hybrid detectors consist of a separate detection and electronics layer in contrast to monolithic detectors (e.g. MAPS, [71]) consisting of a single layer, serving as both detection and electronics. Hybrid detectors allow to optimize the read-out electronics and the sensor separately. They also offer more freedom in the choice of the sensor material and thickness.

Common materials for sensors are silicon, which is widely-used nowadays, gallium arsenide (GaAs) and cadmium telluride (CdTe). Although, the latter have better absorption properties (see figure 3.2), they are either toxic, more difficult to manufacture or have other non-beneficial properties, and are therefore not so commonly used.

In the case of strip detectors, the read-out chip and sensor are glued on a printed circuit board (PCB) as mechanical support. They are electrically connected with wire-bonds, commonly used in chip manufacturing. For high density pixel detectors, the connection is done by bump-bonding. Figure 3.1a shows a schematic view of a hybrid assembly. The transparent volume is the sensor. The bottom layer represents the read-out chip. During the bump-bonding process these two parts are connected mechanically and electrically with indium bumps.

Different processes are used for the bump-bonding. Commercial processes usually use solder bumps. In this thesis the PSI in-house process, initially developed by the particle physics group from R. Horisberger for the CMS pixel detector at CERN, was used. This process uses indium bumps. Figure 3.1b shows a close-up view of a hybrid assembly manufactured at PSI. The sensor, which is bump-bonded to the read-out chip, has a thickness of 320 $\mu$m and is much thinner than the electronics. Also visible are the wire-bonds connecting the read-out chip to the PCB.
Figure 3.1: (a) Schematic view of a hybrid assembly. The transparent volume is the sensor, which is connected with indium bumps to the read-out chip (depicted in yellow). (b) Picture of a hybrid assembly. The read-out chip is glued on a printed circuit board (PCB) and the sensor is bump-bonded on the read-out chip. The array of wire-bonds from the PCB to the read-out chip transfers control and analog signals. One wire is bonded on the backplane of the sensor and supplies the sensor with high-voltage.

Figure 3.2: Sensor efficiency of different materials and two thicknesses for an energy range of 1 to 50 keV. The solid lane represents the efficiency for a 320 µm thick sensor and the dashed line for a 450 µm thick sensor.
3.2 Physics of silicon detectors

In this section the properties of silicon as a detecting material will be discussed. The working principles of microstrip and pixelated detectors will be described and the main issues of sensor design will be pointed out.

3.2.1 Basic properties of silicon

In a semiconductor charge is transported by both, electrons and electron vacancies (holes). The number of intrinsic charge carriers depends on the temperature and on the energy gap between valence and conduction band of the material. In silicon the energy gap is 1.1 eV and the charge carriers concentration is $1.5 \times 10^{15} \, \text{cm}^{-3}$ at room temperature [72].

In pure semiconductor crystals the number of electrons and holes is equal in the conduction band. This balance can be changed by introducing a small amount of impurity atoms having one more (donors) or less (acceptors) electron in their outer atomic shell. The dopant atoms integrate themselves into the lattice and introduce an additional energy level in the forbidden energy gap between the valence and conduction band. The presence of a level inside the forbidden gap shifts the Fermi level of the semiconductor material.

In the case of donors, the level is close to the conduction band, thus creating an excess of conduction electrons. The acceptor level is close to the valence band and causes an excess of holes as charge carriers. A semiconductor doped with donors (n-type semiconductor) has electrons as majority carriers. When the dopant is an acceptor (p-type semiconductor) the majority of charge carriers are holes.

3.2.2 Transport of charge carriers

Charge carriers in a crystal lattice can be considered as free particles with a mean kinetic energy of $\frac{3}{2} kT$, where $k = 8.617 \times 10^5 \, \text{eV \, K}^{-1}$ is the Boltzmann constant and $T$ the absolute temperature [73]. In Silicon, they move randomly with a mean thermal velocity of $10^5 \, \text{m/s}$ at room temperature [73]. Their mean free path, without scattering on the lattice or on impurities, is in the order of 0.1 $\mu$m, while the mean free time is $\tau_c = 10^{-12} \, \text{s}$ [73]. In equilibrium condition their average distance traveled is zero. Two non-equilibrium conditions are now considered. First, if an electric field is present, the charge carriers drift along the field lines. And second, in the presence of a gradient in the charge carrier concentration, we have diffusion.

**Drift** To detect the charge carriers produced by the photon, an electric field is applied, such that the charge carriers drift along the field lines towards the read-out electrodes. The direction is opposite for electrons and holes. In the presence of an external electric field the charge carriers are accelerated between two random collisions [73]. The direction of the drift is given by:

$$
\begin{align*}
v_n &= \frac{e \tau_c}{m_n} E = -\mu_n E \quad \text{for electrons,} \\
v_p &= \frac{e \tau_c}{m_p} E = \mu_p E \quad \text{for holes,}
\end{align*}
$$

(3.1)

where $v$ is the velocity, $m$ is the effective mass of electrons (holes), and $E$ is the applied electric field. The above formula is valid for weak electric fields. If the field is stronger the charge carriers...
will interact with the lattice and a maximum drift velocity will be reached. This can be explained with the Drude model [74]. The drift current is given by:

\[
\begin{align*}
J_{n,\text{drift}} &= -en\mu_n E \\
J_{p,\text{drift}} &= ep\mu_p E
\end{align*}
\]

(3.2)

where \( n \) and \( p \) are the carrier concentrations.

**Diffusion**  The spread of charge carriers (electron or holes) in the absence of an electric field is called diffusion. In the case of a gradient in the carrier concentration, a movement of charge carriers is more probable in the direction of regions with low concentration [73]. The current of the diffusion per unit area is given by

\[
\begin{align*}
J_{n,\text{diff}} &= -\frac{kT}{e}\mu_n \nabla n \\
J_{p,\text{diff}} &= \frac{kT}{e}\mu_p \nabla p
\end{align*}
\]

(3.3)

where \( e \) is the elementary charge, \( \nabla n \) and \( \nabla p \) are the gradients of the electron and hole concentration, and \( \mu_n = 1415 \pm 46 \, \text{cm}^2 \, \text{V}^{-1} \, \text{s}^{-1} \) and \( \mu_p = 480 \pm 17 \, \text{cm}^2 \, \text{V}^{-1} \, \text{s}^{-1} \) are the electron and hole mobilities at 300 K, respectively [75]. The mobilities \( \mu_n \) and \( \mu_p \) are a function of \( \tau_c \) and are therefore dependent on the temperature. Diffusion is the main reason for charge sharing between sensor pixel or strips. Charge sharing is revisited and explained in more detail in section 3.3.

### 3.2.3 Silicon sensor

A silicon sensor works usually like a reverse biased p-n junction. An impinging photon interacts with the sensor and generates electron-hole pairs. The required energy for generating one electron-hole pair is about 3.6 \( \text{eV} \) for silicon, while about 20 \( \text{eV} \) is required for gas ionization and therefore a much better energy resolution can be reached with silicon sensors [73].

**p-n junction**  Figure 3.3a is a sketch of a p-n junction. A p-n junction is a boundary of p-type and an n-type semiconductor on a single crystal. In such a configuration, the free electrons of the n region close to the junction diffuse into the p region and recombine with negatively charged ions in the p region, leaving positively charge ions in the n region. The holes act in an opposite way. I.e. from the p region they diffuse into the n region, leaving negatively charged ions in the p region. They recombine in the n region forming positive ions. This results in a region near the junction depleted from charge carriers, as shown in figure 3.3b and c. This region is known as the depletion region, or space charge region.

The charge distribution in the depletion region creates an electric field (see figure 3.3d), which excites an opposite force on the charge carrier, compared to the diffusion. Therefore, once the force of the diffusion and the electric field on the charge carriers cancel out, the depletion will reach an equilibrium. The electric field will also create a potential difference, known as contact potential (see figure 3.3e). The contact potential of common semiconductors is around 1 V.

The depletion depth can be tuned by applying an external potential to the sides of the junction. If a positive potential is applied to the p-type side and a negative potential is applied to the n-type side (known as forward bias), the depletion region will decrease until the junction behaves like a conductor. If a negative potential is applied to the p-type end and a positive potential is applied to
3.2. PHYSICS OF SILICON DETECTORS

Figure 3.3: (a) A p-n junction and plots of (b) charge carriers concentration, (c) charge density distribution, (d) electric field and (e) electric potential as a function of the distance from the junction [76].

the n-type end of the junction, the p-n junction is operated in reverse bias. In this configuration, the holes in the p-type material (and the electrons in the n-type material) are pulled away from the junction, causing an increase of the size of the depletion region. In the sensor the n and p doping concentration are usually very different. The read-out electrodes are heavily doped and the bulk only slightly. In this configuration the electrodes are only very little depleted, while the bulk is fully depleted.

Bias voltage An applied potential (bias voltage) generates an electric field, which accelerates the charged particles towards opposite electrodes in the depleted region of the sensor. The charges drift at a speed which depends on the electric field but saturates at values $\sim 10^7 \text{ cm/s}$ for fields close to $10^4 \text{ V/cm}$ [73]. The bias is usually chosen so that, the depletion region extends throughout the silicon bulk in order to maximize the size of the region, that is sensitive to radiation and to reduce the noise. For example, a 300 $\mu$m thick n-type silicon sensor with a resistivity of 4.5 $k\Omega \text{ cm}$ fully depletes at 65 V bias voltage [73].
CHAPTER 3. X-RAY HYBRID SEMICONDUCTOR DETECTORS

Dark current  The holes are constantly removed out of the depleted region by the field in the junction, thus generating a small current, known as dark current [73]. The carriers are generated thermally, and therefore the current depends on the temperature. It also depends on the thickness of the sensor and the depletion. For a charge integrating detector the dark current is also accumulated during the integration time. To account for this a dark image is acquired. A dark image is an acquisition without exposing the sensor to X-rays. This image can be used to measure the contribution from the dark current. The dark image is subtracted from the actual image, to have a dark current corrected result.

Generation of charge carriers  If a photon interacts with the semiconductor a photo-electron will be produced. While the photo-electron travels through the lattice, the energy of the photo-electron produces electron-hole pairs (charge carriers). On average, 1 electron-hole pair is generated per $c_{Si} = 3.6 \, \text{eV}$ of energy deposited [73]:

$$<n> = \frac{E_{ph}}{c_{Si}},$$  \hspace{1cm} (3.4)

where $<n>$ is the expected value of the amount of electron-hole pairs produced, $E_{ph}$ is the energy of the photon and $c_{Si}$ is the conversion coefficient for Si. The variance of $n$ is reduced compared to the statistical variance by the Fano factor. See a more detailed explanation about Fano noise in section 2.3.2.

3.3 Charge sharing

During the drift, the charge cloud also diffuses and when its size becomes comparable with the channel or pixel pitch $p$ or the photon is absorbed in a region between adjacent channels or pixels, it can be partially collected by multiple channels, giving rise to the so called charge sharing [77]. For a 320 $\mu$m thick silicon sensor with a bias voltage of 120 V, the charge sharing distance was measured to be $d = 17 \pm 3 \, \mu m$ [52]. For the photon based position interpolation methods, explained in chapter 4, the charge sharing effect is essential. Charge sharing depends on many parameters, namely the X-ray energy, the sensor geometry (including thickness, pixel pitch and the electric field) and on the sensor material. Therefore, accurate simulation considering all parameters are difficult. [77] presents a simplified model for calibrating detectors, where the effects of charge sharing are significant. With this model it was possible to perform the energy calibration for small strip and pixel detectors and to better understand the charge sharing effect for the interpolation methods.

In figure 3.4a the model for the charge sharing between strips of a one-dimensional detectors is depicted. For strip detectors, the model defines two regions. In the center region, with a size of $(p - d)$, around the channel electrode, the generated charge is fully collected by one pixel. In the border region, the charge is partially collected by adjacent strips. The model assume that the charge sharing is linearly dependent on the distance between the strips.

For pixelated detectors, figure 3.4b shows the model for the charge sharing between square pixels of size $p \times p$. The charge collection efficiency is 100 % in the center region. This region has a size of $(p - d)^2$. Outside this region, the charged is linearly shared with the neighbor pixels. Therefore, at the physical pixel border 50 % of the charge are shared with a neighboring pixel and at a distance of $(p + d)/2$ from the pixel center the charge collecting efficiency of the considered pixel is zero.
Figure 3.4: Simple model of charge sharing behavior. (a) is the model for a strip detector with strip pitch \( p \). Towards the channel border the collection efficiency (solid line) decreases, since it is shared with the adjacent channels (dashed lines). (b) shows the model for a pixelated detector. The solid black line indicates the pixel border of a pixel with pitch \( p \times p = 25 \times 25 \text{ \( \mu \text{m} \)}^2 \). In the region \( d \) around the pixel border, the charge is only partially collected by the center pixel. Some charge is collected by the neighboring pixels.

For pixel detectors, the model assumes, that each pixel can be divided in a region, where no charge sharing with neighboring pixels occurs (center region), where charge sharing with one neighboring pixel occurs (border region), and where charge sharing with three neighbors occurs (corner region). It further assumes, that if a photon is absorbed in the region, where charge sharing between pixels occurs (i.e. border and corner regions), the charge is shared linearly between the two or four neighboring pixels (see figure 3.4b). Likewise for the strip detectors. In the border region, the charge is shared linearly with the adjacent channel.

If \( p \) is the pixel or channel pitch and \( d \) is the size of the charge cloud, after drift and diffusion, the parameter \( \alpha \) is defined as [77]:

\[
\alpha = \frac{d}{p}.
\]  

(3.5)

The area of the two regions of the strip detectors, are defined by using the parameter \( \alpha \) in the strip model (SM):

\[
A_{SM} = \frac{(1 - \alpha)}{(1 + \alpha)}; \quad B_{SM} = \frac{2\alpha}{(1 + \alpha)},
\]

(3.6)

where \( A_{SM} \) is the center region and \( B_{SM} \) is the border region.

The area of the three regions for the pixel model (PM) can now be expressed as ratio between pixel size and charge cloud, i.e. as a function of \( \alpha \):

\[
A_{PM} = \frac{(1 - \alpha)^2}{(1 + \alpha)^2}; \quad B_{PM} = 4\frac{\alpha(1 - \alpha)}{(1 + \alpha)^2}; \quad C_{PM} = 4\frac{\alpha^2}{(1 + \alpha)^2},
\]

(3.7)
where $A_{PM}$ is the center region, $B_{PM}$ is the border region and $C_{PM}$ is the corner region. Note that
\[
A_{SM} + B_{SM} = 1 \quad \text{and} \quad A_{PM} + B_{PM} + C_{PM} = 1.
\]
Therefore, these parameters are the ratio of the area where a particular charge sharing behavior dominates.

The charge collecting efficiency for the SM is:
\[
Q_{SM}(x) = \begin{cases} 
  Q_0 & \text{if } x \in \text{center} \\
  Q_0 \frac{p+d-2|x|}{2d} & \text{if } x \in \text{border}
\end{cases},
\]
where $Q_0$ is the total charge deposited by the photon and $x$ is the distance to the pixel center.

The charge collecting efficiency for the PM is:
\[
Q_{PM}(\vec{s}) = \begin{cases} 
  Q_0 & \text{if } \vec{s} \in \text{center} \\
  Q_0 \frac{p+d-2|x|}{2d} & \text{if } \vec{s} \in \text{vertical border} \\
  Q_0 \frac{p+d-2|y|}{2d} & \text{if } \vec{s} \in \text{horizontal border} \\
  Q_0 \left(\frac{p+d-|y|}{d} - \frac{|x|}{d}\right) & \text{if } \vec{s} \in \text{corner}
\end{cases},
\]
where $\vec{s} = (x,y)$ is a two-dimensional position vector with origin at the pixel center.

The theoretical spectrum $\hat{S}_{SM}(E)$ and $\hat{S}_{PM}(E)$, respectively, can be derived from the charge collecting efficiency, by converting the collected charge to the X-ray energy $E = Q3.6 \text{ eV}$, and by a change of variable. If the distribution of photons is uniform over the entire detector, a change of variable can be obtained by inverting and differentiating the function $Q_{SM}(x)$ and $Q_{PM}(\vec{s})$, respectively:
\[
\hat{S}_{SM}(E) = N_0 \left\{ A_{SM} \delta(E - E_0) + B_{SM} \Theta(E_0 - E) \right\},
\]
and
\[
\hat{S}_{PM}(E) = N_0 \left\{ A_{PM} \delta(E - E_0) + B_{PM} \Theta(E_0 - E) - C_{PM} \ln \left(\frac{E}{E_0}\right) \Theta(E_0 - E) \right\},
\]
where $\delta$ is the Dirac delta function and $\Theta$ is the Heaviside step function and $N_0$ is the amount of detected photons.

The measurable spectrum $S_{SM}(E)$ and $S_{PM}(E)$ can be obtained from the theoretical spectrum of equation 3.11 and equation 3.12, by convoluting each contribution with the Gaussian noise $\sigma$. The Dirac delta function convoluted with Gaussian noise results in a Gaussian itself, while the convolution of the Heaviside step function with noise results in an error function (denoted erf).

Finally, the spectra produced by this model is the sum of the three regions normalized by their sizes, convoluted with the noise of the detector $\sigma$ and scaled by the amount of detected photons.
3.3. **CHARGE SHARING**

\[ N_0: \]

\[
S_{SM}(E) = N_0 \left\{ \frac{A_{SM}}{\sigma \sqrt{2\pi}} \exp \left[ -\frac{(E - E_0)^2}{2\sigma^2} \right] + B_{SM} \frac{1 - \text{erf} \left( \frac{E - E_0}{\sigma} \right)}{2E_0} \right\}, \tag{3.13}
\]

and

\[
S_{PM}(E) = N_0 \left\{ \frac{A_{PM}}{\sigma \sqrt{2\pi}} \exp \left[ -\frac{(E - E_0)^2}{2\sigma^2} \right] + \frac{1 - \text{erf} \left( \frac{E - E_0}{\sigma} \right)}{2E_0} - C_{PM} \ln \left( \frac{E}{E_0} \right) \frac{1 - \text{erf} \left( \frac{E - E_0}{\sigma} \right)}{2E_0} \right\}, \tag{3.14}
\]

where \( E \) is the signal amplitude, and the fit parameters are \( E_0 \) representing the X-ray energy of the monochromatic beam, \( \sigma \) is the electronic noise.

Figure 3.5: Theoretical spectrum derived from equation 3.13 (a) and equation 3.14 (b), respectively. The parameters are \( \alpha = 70 \% \), \( E_0 = 10 \text{ keV} \) and \( \sigma = 300 \text{ eV} \). In (a) are two contributions from the center and the border region. In (b) are the 3 contributions visible: from the center of the pixel (where no charge sharing occurs), from the border, and from the corner. The sum of all contribution is shown in blue.

Figure 3.5b shows a theoretical spectrum generated with the model shown in equation 3.14. The beam energy \( E_0 \) is 10 keV, and the error contribution from the detector is 3 %, while an \( \alpha \) of 70 % was assumed. The contribution of the pixel center (cyan line) is a Gaussian distribution with standard deviation of the electronic noise. The contribution of the border (green line) is an error function with the inflection point at \( E_0 \) and a \( \sigma \) of the electronic noise, and the corner contribution is also an error function scaled with the logarithmic ratio of the signal amplitude and the X-ray energy. At the beam energy the total spectrum (blue line) is dominated by the contribution of the center, and at low energies (below \( \sim 6 \text{ keV} \) in this theoretical spectrum) the corners have the biggest contribution.
3.4 Detection of generated charge

After the charge is generated in the sensor and collected at the anode, it is amplified and detected by an electronic circuit. While the first part after the electrode of the pixel or channel is always an amplifier, there are two major methods to detect the amplified signal. The two methods are explained in more detail in this section.

3.4.1 Single photon counting detectors

The front-end of single photon counting detectors is designed, such that the charge of each absorbed photon will generate a voltage pulse at the output of this stage. This is achieved by a pre-amplifier in combination with one or two shapers, as depicted in figure 3.6. They are configured such that they produce a fast peak voltage. The peak voltage is proportional to the generated charge and therefore to the energy of the absorbed photon. The height of the peak voltage \( V_{in} \) is compared with a comparator to a global threshold voltage \( V_{th} \), which is common for all channels. If the input voltage \( V_{in} \) exceeds \( V_{th} \) a digital counter is incremented.

Between the counter and the comparator a pulse former is also present. This pulse former guarantees a minimal pulse length, so that the counter will recognize the signal and increment its value. \( V_{th} \) has to be carefully calibrated with different known monochromatic X-rays. This can be done by scanning the threshold voltage and observe the count values for a monochromatic X-ray beam. The so called S-curve plot, where the counts versus the threshold voltage is plotted, allows to investigate at what voltage the counts increase significantly. At this voltage the count efficiency and the count rate are in a optimum.

The MYTHEN detector, depicted in figure 3.6, has additional trim bits for each channel. These trim bits allow to calibrate each channel separately to account for channel-to-channel variations of the gain of the front-end stage, i.e. pre-amplifier and shapers.

To have small dead-time after a photon detection, the pre-amplifier and the shaper have to produce a narrow peak. This is achieved by the two shapers after the pre-amplifier, which act as differentiating circuits. If the signal after the first detection does not fall below \( V_{th} \) and a new photon arrives it will not be counted. This so called pile-up can be a major limit in the count-rate capability of such a detector.

After the acquisition, the binary counters are read out in serial fashion and are resetted for the next acquisition. Photon counting detectors are limited in the minimal pixel size, since the charge sharing effect (see section 3.3) leads to partial charge collection at several channels, and the signal does no exceed \( V_{th} \) in any of these channels. Post-processing of data acquired by photon counting detectors is relatively simple, since they produce a binary value, corresponding to the number of photons detected.

3.4.2 Charge integrating detectors

Charge integrating detectors are mainly developed to overcome the limits of photon counters in combination with free-electron lasers (FELs). In FELs, the incident photons of a bunch arrive all at the same time (i.e. in femto seconds). The front-end of photon counting detectors operates in the order of nanoseconds, and therefore photon counters can only count 1 photon in this time frame. More photons in a pixel would create a pile-up in the analogue part and could not be counted.

Charge integrating detectors can solve this problem by not relying on a separate signal peak
3.4. DETECTION OF GENERATED CHARGE

for each photon, but by integrating the total charge produced in a sensor pixel on a capacitor. The charge integrating pre-amplifier is designed, such that it amplifies the signal and stores it on a storage capacitor. After the integration time (exposure time), the charge stored on the capacitor is read-out in an analog fashion and further amplified, before an analog-digital converter digitizes the value. The digitized value can then be back-calibrated to the number of monochromatic photons, or in the case of a polychromatic source, to the total x-ray energy absorbed in the integration time. For different applications, the requirements for the gain, i.e. the voltage difference in the capacitor in relation to the absorbed charge, can differ quite a lot. For example in FEL experiments, one would like to detect single 12 keV photons per pixel, but also photon intensities of $10^4$ 12 keV photons. Therefore, charge integrating detectors can be equipped with dynamic gain switching, where an additional charge capacitor is connected to the amplifier, if the voltage on the feedback exceeds a certain limit [12].

Figure 3.7 shows the signal response of a JUNGFRAU pixel if the input charge is scanned. JUNGFRAU has three different gains. The points, where the dynamic gain switching logic changes gain are indicated with a dashed red line. In the high gain mode the signal level (i.e. the ADC value) differs significantly for the different photon counts. The gain switching to the medium gain happens at an equivalent charge of $\sim 30$ 12 keV photons. The high gain is selected if more than $\sim 800$ 12 keV photons are detected. The total dynamic range of one JUNGFRAU pixel is $\sim 10^4$ 12 keV photons, which is in agreement of the expected flux at the SwissFEL. The sign of the slope of the medium and the low gain is reversed, due to bypassing of the correlated double sampling (CDS) stage after switching to a higher gain. The CDS stage reduces the noise introduced by the release of the reset switch. This is achieved by performing an analogue subtraction of the output signal of the preamplifier after releasing the reset switch.

Another interesting application for charge integrating detectors are low flux applications. If the photon flux and the exposure time are tuned, such that the average occupancy is lower than one photon per channel (pixel) and exposure, it is possible to extract additional information per photon. First, the deposited charge can be related to the photon energy for each photon. Second, by exploiting the charge sharing effect, the charge ratio between adjacent pixels can be back-propagated to the absorption position of the photon. In this thesis, this so called, single-photon regime of charge integrating detectors is used to perform experiments, where high spatial resolution

Figure 3.6: Channel architecture of the MYTHEN photon counting detector [78].
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Figure 3.7: Signal response of the JUNGFRAU detector, at different input charge [16]. This detector has three different gain levels, which are switched dynamically during the acquisition.

or photon energy information is required.

3.5 Strip detector GOTTHARD

GOTTHARD (Gain Optimizing microsTri p sysTem witH Analog ReaDout) is a one-dimensional detector system based on the principle of charge integration with automatic gain switching capability [12, 50]. The detector module is composed of 10 readout ASICs (Application Specific Integrated Circuits), that are wire bonded to a single 300 μm thick silicon sensor for a total of 1280 channels. The read-out electronics is capable of reading all the 1280 channels at 40 kHz, or allows to specify a small region-of-interest (256 channels), which then can be read-out at higher frame rates (140 kHz) [50].

GOTTHARD features 4 different gains depending on the requirements. The low gain mode has a dynamic range of $10^4 \times 12$ keV photons, while the very high gain has a dynamic range of only $\sim 40 \times 12$ keV photons but an ENC noise as low as $\sim 150$ $e^{-}$ (rms). GOTTHARD is capable of dynamic gain switching, however, this feature was not used during the experiments conducted in this thesis. Instead, the detector was always operated in very high gain mode.

Each channel has its own read-out electronic on the ASIC, designed in IBM 130 nm CMOS technology, depicted in figure 3.8. After the sensor, the front-end block based on an inverting preamplifier integrates the charge produced in the sensor. In the beginning of the acquisition the reset switch is released and the charge starts to accumulate in the capacitor $Cf1$. Depending on the currently selected gain, the charge is shared between $Cf1$, $Cf2$ and/or $Cf3$. If GOTTHARD operates in the automatic gain switching mode, the gain switching logic is engaged and adds more capacitance, once the signal of the capacitor exceeds a certain threshold. Additionally to the CDS
stage, each channel has a channel buffer, that refreshes the signal before the analog to digital conversion. The analog signal of 32 channels is multiplexed serially on the chip and fed into an external ADC [12].

Figure 3.9 shows the interior of the GOTTHARD multi-pitch module. The sensor is glued at the edge of the PCB. This sensor has 10 groups of channels with different strip pitches. Each group is connected to one read-out chip (ROC). Each ROC has 128 channels. The ROCs are also glued on the PCB and connected to the sensor and the PCB with wire-bonds. The read-out electronics has 5 ADC chips, which are visible at the top of figure 3.9. Each ADC chip has 8 channels. To read-out the integrated charge after the acquisition, the analog signals of 32 detector channels are multiplexed one-by-one to one ADC channel. The X-rays enter the detector from the entrance-window visible below the sensor.

For the experiment in this thesis, a sensor with groups of strips with different pitches ranging from 10 µm to 200 µm and a length of 2.1 mm was used (see figure 3.10). The small pitch strips are connected to the 50 µm pitch wire-bond pads by fan-out lines (indicated in green), which increases the input capacitance. In particular the behavior of the 25 µm pitch strips was investigated, which are organized in two groups of 64 channels giving each a field of view of 1.6 mm [50].

3.6 Pixel detector MÖNCH

MÖNCH (Micropixel with enhanced pOsition rEsolution usiNg CHarge integration) is a charge integrating hybrid pixel detector with a pixel size of 25µm × 25 µm. To evaluate the performance of this small pixel detector in different scopes of applications, the SLS Detector Group developed 5 different pixel architectures organized in 4 super-columns (the fourth super-column is further divided and consists of two different type of pixels) [53]. Figure 3.11b shows the prototype read-out chip, an ASIC designed in UMC 110 nm technology. Also depicted are the 4 super-columns (in yellow) and the read-out pads (red regions). The sensor depicted in figure 3.11a is bump-bonded to the top left corner of the read-out chip. Two pixel architectures have statically selectable
Figure 3.9: Design of the multi-pitch GOTTHARD module. On the top the PCB with 5 ADCs is visible. 10 read-out-chips (ROCs) are glued at the bottom of the PCB and electrically connected to the PCB and the sensor. The multi-pitch sensor is divided in 10 sections with different strip pitches starting from 10 μm up to 200 μm. The total sensor width is 6.4 mm.

Figure 3.10: A close-up of a region of the multi-pitch GOTTHARD sensor. The small pitch channels are grouped in either 128 channels (for the 10 μm pitch channels) or two times 64 channels. To connect the channels (yellow) to the wire-bond pads (blue) a fan-out was designed (green). A group of 25 μm channels has a field-of-view of 1.6 mm.
3.7 Acquisition system for MÖNCH and GOTTHARD

The standard detector acquisition system, that is used for all detectors developed at PSI, consists of various software and hardware components. Figure 3.13 gives a brief overview of the system.

Each pixel has analog electronics responsible for charge integration and signal preparation for off-pixel transfer (see figure 3.12). The front-end block directly, which is connected to the sensor, is a charge sensitive amplifier, that integrates the charge on a feedback capacitor. One additional capacitor can be switched in the feedback loop to obtain two different gains. The signal gain in high gain mode is a factor of 4 higher than in low gain mode [50]. Consequently, the dynamic range is diminished by this factor. A CDS stage follows, to reduce the low frequency noise contributions coming from the preamp and its reset transistor [79]. Each pixel has a storage cell, that allows to store the signal after the acquisition until the read-out. During read-out the signal is amplified in the pixel and on the off-chip buffer, that is common for 40 columns. At the end of each integration time, the pixel rows are selected successively and the signal levels are transmitted to read-out buffers [50]. An analog-to-digital converter transforms the voltages, that represent the signal values, at a rate of 10 Mpixels s\(^{-1}\).

With low read-out noise and a fast data acquisition (DAQ) system, the architecture is optimized for single photon detection, high position resolution and photon energy discrimination at synchrotrons and X-ray tubes. Further details about the chip specification, the architecture of all the 5 different pixel types and the analog read-out chain can be found in [79, 50].

Figure 3.11: (a) front-side of the sensor for MÖNCH. The field-of-view is 4 × 4 mm\(^2\) and it has 25600 pixels. (b) shows the read-out chip of MÖNCH. It has a size of 5 × 5 mm\(^2\). The red rectangles indicate the wire-bond pads. The ROC has 5 different pixel architectures grouped in 5 super-columns (named SC1 to SC4B).

preamplifier gains and target synchrotron applications. The current prototype has a field of view of 4 mm × 4 mm, and a total of 25600 pixels. In this thesis, the first super-column with a pixel architecture optimized for single photon imaging was used. The field of view of this super-column is 1 mm × 4 mm.
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Figure 3.12: Diagram of the pixel architecture of MÖNCH.

**Hardware architecture** The read-out board has three major digital components. The CPU is connected with a 100 MBit connection to the computer network and controls the field-programmable-gate array (FPGA). The analog digital converters (ADC) convert the analog amplified signal from the read-out chip into a digital signal with 14 bit dynamic range. The FPGA has two purposes. First, it receives the acquisition parameters from the CPU and controls the read-out chip. Second, it receives the digitized data from the ADCs and sends it over a fast Ethernet connection.

A server, equipped with a fast Ethernet connection, receives the data and prepares it for storage and for a live view. The acquisition is controlled with a conventional computer that is connected to the CPU of the detector and to the server, that is receiving the data.

For data-transfer between detector and receiver either a 1 or 10 GBit Ethernet connection is used. For the configuration paths 100Mbit Ethernet is sufficient.

**Software architecture** The acquisition system, a client-server system, is controlled by the client software running on a PC, which is operated by the user and comes with a text or graphical user interface. The text version is mainly used for scripting purposes and allows automation of measurements. The client software sends control sequences to the server-software, running on the CPU of the detector. The server-software reconfigures the FPGA by changing the configuration registers over an internal dedicated link in the detector. In the firmware of the FPGA a state machine is running, that controls the read-out chip under consideration of the configuration given by the user. The client-software also controls the receiver, i.e. storage location and online post-processing parameters. The detector data is directly transmitted from the FPGA firmware to the receiver-software running on a server-machine, which will post-process the data. This involves for once storage of the data, but also preparation of a live view on the client software.

**Data output format** The Ethernet transfer protocol limits the amount of data per packet to 1500 bytes (if jumbo-packets are not enabled), and therefore the amount of pixel data per packet is limited to 750 (assuming a dynamic range of 16 bit). Therefore, the FPGA segments each acquired frame into several network packets. For the GOTTHARD system with 1280 channels per frame, the frame is divided in two packets, each containing 640 channel values.

The current MÖNCH prototype has a total of 160k Pixels. The pixel values of one frame are divided in 40 network packets. Each super-column is divided in 10 networks packets, with 16 rows
3.7. ACQUISITION SYSTEM FOR MÖNCH AND GOTTHARD

Figure 3.13: The data acquisition and controlling system for the MÖNCH and GOTTHARD detector. A micro Linux system receives the control signals from a client software (text or graphical user interfaces are available) operated by the user and sets the state machine control register in the FPGA. The FPGA transmits digitized sensor data over a fast network link to the receiver for storage.

and 40 columns of pixels (see figure 3.14).

The firmware of the FPGA gives the network packets consecutive 32-bit numbers. For GOTTHARD the least significant bit (LSB) indicates the packet of the frame, i.e. the first 640 channels are in the packet with LSB = 0 and the second part has LSB = 1. The rest of the bits of the packet number identifies the frame number. For MÖNCH, the least significant byte identifies the packet number, and is used to reconstruct the full frame in the receiver. The packet numbers from 40 up to 255 of the packet identifier are not used for MÖNCH.
Figure 3.14: MÖNCH frame segmentation: The 160 pixel $\times$ 160 pixel of MÖNCH are divided in 4 super-columns (SC1 to SC4). For each supercolumn 10 Ethernet packets containing 40 pixel $\times$ 16 pixel are transmitted.
Chapter 4

High resolution imaging

In this chapter, the acquisition process for energy dispersive imaging and position interpolated imaging with small-pitch strip and pixel charge integrating detectors is explained. First the concept and advantages of operating a charge integrating detector in the single photon regime is addressed. Then the acquisition system of MÖNCH and GOTTHARD and also the data-processing after the acquisition is discussed. One of the proposed methods is tested in depth with simulation to demonstrate its capabilities. Parts of this section are a reprint of the publications: [50], [53].

4.1 Concept

In conventional x-ray image acquisition methods the pixel intensity is proportional to the absorbed number of photons and their energy. The gained information is reduced to the integrated count of photons per pixel in the case of a monochromatic beam. In the case of a poly-chromatic beam the photon count is convoluted with the deposited energy spectrum and a back calibration of the resulting intensity to the amount of photons is no longer possible. Normally, high energy photons have a higher weight in the image but carry less contrast information, since a big fraction of them penetrates the sample unaffected.

A first step towards gaining more information per photon where photon counting detectors. These detectors implement a simple energy discrimination by applying one or several thresholds and only counting photons with a higher energy than the thresholds. By acquiring multiple exposures with different thresholds or reading out the counter of the different thresholds, it is possible to extract a spectrum of the detected photon beam. These type of detectors have the advantage, that they are easy to use, they suppress the low-frequency noise (including dark current) and they have a linear counting behavior over their entire dynamic range [80]. One major disadvantage of the photon counting detectors, is that they have a limited count rate, since the electronics has a recovery time after a photon is detected. This is especially a problem for free electron laser experiments, where all photons of a bunch arrive simultaneously. Therefore, new detectors that surpass that limitation were developed.

This new generation of detectors, i.e. charge integrating detectors, are capable to detect many photons simultaneously, and are therefore suitable for free electron laser experiments. Each pixel or strip has a integration capacitor, where the cumulative charge of all arriving photons in a integration window is stored. After reading out the charge value, a back-calibration to the amount of photons is possible. Additionally, if only one x-ray photon is captured per integration window, it is possible to determine the energy of the photon [12]. To gain this additional information, the
exposure time and photon flux is reduced, such that less than one photon is detected per pixel and per exposure on average. If environmental conditions (e.g., source and sample) remain constant over the experimental time it is possible to aggregate the information of many such short-exposures (sub-frames). This results in the same measured intensity as performing a single long exposure. This acquisition process is called single-photon regime.

Operating the detector in the single-photon regime has several advantages. First, for each photon the absorbed charge can be determined and therefore energy resolving detection is possible. Second, while the produced charge of one photon absorption drifts towards the read-out implant it spreads on multiple pixels. By analyzing the detected charge ratio of a pixel cluster (i.e., the pixels absorbing charge from one photon) a finer position resolution than the physical pixel pitch can be achieved. Therefore, by operating the detector in the single-photon regime and analyzing each photon event separately, it is possible to produce a high resolution image with a finer virtual-pixel size than the physical pixel size of the detector.

To extract this additional information (i.e., energy and position) for each photon the data needs to be processed after the acquisition. The determination of the energy requires an energy calibration, i.e., the measurement of the response of the detector to different photon energies. Similarly, the determination of the interpolated position requires a calibration of the detector response to different incoming photon positions. This is done by acquiring a flat illumination, i.e., a homogeneous illumination without sample and extracting the calibration constants from this acquisition. Figure 4.1 shows an overview of the data processing. The flat acquisition consisting of many sub-frames with a flat illumination across the detector is needed for the calibration of the interpolation algorithm and for the flat-field correction after the image interpolation. For both acquisitions the photon finder first extracts the photon events from many individual sub-frames. In a second step, the calibrated image interpolator generates the high resolution image from the second acquisition. After that step, the flat-field correction can be applied. Note that after the energy calibration the information extracted from the photon finder also contains the information about the energy of the photon.

![Diagram of data processing](image.png)

**Figure 4.1:** Overview of the processing of single-photon regime data. The first step after the acquisition is the extraction of photon events from the sub-frames. The events of a flat acquisition are fed into the calibration process of the position interpolation algorithm. After that an image is acquired and the extracted events are processed by the position interpolation algorithm.

### 4.2 Photon-finding algorithm

The analog read-out chain of charge integrating detectors introduces noise to the signal and integrates dark current during exposure. In the read-out signal this shows up as a signal pedestal,
which is dependent on exposure time and sensor conditions, and a Gaussian-shaped noise on top of the pedestal value [50].

A simple way to remove the signal pedestal is to acquire dark-images without illumination and subtract the average signal levels from the recorded photon data. The disadvantage of this method is that during long data acquisition the pedestal can drift (e.g., by temperature changes) [50]. Therefore, tracking the pedestal over time is beneficial. If all pixels, that are not part of a cluster, are considered as a part of the dark-image, they can be used to update the pedestal as a moving average. In this chapter a cluster-finding algorithm for strip and pixel detectors, that discriminates according to noise and pedestal is presented.

For a one dimensional dark-image corrected frame, where the collected charge of channel \( i \) is \( Q_i \), a cluster, i.e., a group of pixel containing a photon hit, is defined when

\[
Q = \sum_{i-i-\left\lfloor \frac{k}{2} \right\rfloor}^{i+\left\lceil \frac{k}{2} \right\rceil-1} Q_i > \sqrt{k \sigma_i},
\]

where \( k \) is the cluster size, \( \sigma_i \) is the ENC of channel \( i \), \( c \) is the threshold and \( Q \) is the total cluster charge [50]. Note that if equation 4.1 yields more than one cluster within \( k \) neighbors, only the one with the highest center value (i.e., highest \( Q_i \)) is extracted. The actual value of the parameter \( c \) is a compromise between efficiency and false positive events and is usually between 3 and 5. This means that the total cluster charge must be at least 6 to 10 times larger than the electronic noise to be detected, similar to single photon counting systems.

The algorithm defined in 4.1 can find up to \( k \) clusters for one incident photon (i.e., one for each channel in a cluster). To prevent this, clusters are rejected if there is another cluster with a higher center value (\( Q_i \)) present within \( k \) neighboring channels.

For a two dimensional dark-image subtracted frame, where the charge of the pixel in row \( i \) and column \( j \) is \( Q_{i,j} \), a cluster has to satisfy the following condition:

\[
Q = \sum_{i-i-\left\lfloor \frac{k}{2} \right\rceil}^{i+\left\lceil \frac{k}{2} \right\rceil-1} \sum_{m=j-\left\lfloor \frac{k}{2} \right\rceil}^{j+\left\lceil \frac{k}{2} \right\rceil-1} Q_{l,m} > k c \sigma_{i,j}.
\]

In this case \( k \) equals 2 for a \( 2 \times 2 \) cluster, i.e., the cluster size is \( k^2 \). Similar to the one dimensional algorithm, only the most significant cluster (highest cluster center \( Q_{i,j} \)) within \( k^2 \) pixels is preserved for further treatment.

### 4.3 Position interpolation algorithms

For the detectors used in this thesis the pixel size is such that the total charge is collected in 2 strips or a \( 2 \times 2 \) pixel cluster (i.e., \( k = 2 \)). Therefore only 2 channels (for the strip detectors) are used for the interpolation. For the two-dimensional pixel detector the average of 2 channels in \( x \) are used to interpolate the \( y \)-coordinates and vice versa for \( x \).

#### 4.3.1 One-dimensional \( \eta \)-algorithm

Assuming a cluster at channel \( l \) and \( l+1 \) has been found, then the charge on the left strip is \( L = Q_l \) and the right strip is \( R = Q_{l+1} \). Assuming, strip \( l \) is at position 0 and strip \( l+1 \) at
position 1 then the linear interpolated position $\eta$ is:

$$\eta = \frac{R}{L + R}.$$  \hspace{1cm} (4.3)

However, $\eta$ is not a linear function of the absorption position of the photon and the interpolated position has to be corrected. Figure 4.2 shows the distribution of $\eta$, for a uniform distribution of photons. Note that a large fraction of the $\eta$ values are between 0 and 1. Unlikely events with values outside of this range can appear, if the photon is absorbed close to the center of one of the electrodes, causing a low signal on the neighbors, and the noise term added by the electronics is negative for one of the strip readings. Additionally, one would expect the peaks in figure 4.2 to be at exactly $\eta = 0$ and $\eta = 1$, since they indicate, that the charge is completely collected by either the left or the right strip. The peaks are slightly shifted to the center, since neighboring strips have a capacitive coupling. I.e. if a strip has a higher signal, the signal level of its neighbors will also increase slightly. This effect is called inter-strip capacitance.

This distribution can be used to correct the interpolated position to obtain the real position \[81\]. The corrected distance $x_{\text{sub}}$ of the pixel center with charge $Q_i$ to the photon hit position can be derived from the previously calculated $\eta$-value:

$$x_{\text{sub}}(\eta_i) = p \int_{-\infty}^{\eta_i} \frac{dN}{d\eta} d\eta,$$  \hspace{1cm} (4.4)

where $p$ is the strip pitch and $\frac{dN}{d\eta}$ is the normalized $\eta$ distribution of a flat illuminated data set (i.e. $\int_{-\infty}^{\infty} \frac{dN}{d\eta} d\eta = 1$). The algorithm defined in equation 4.4 linearizes the position response of the system at the cost of resolution.

Position reconstruction with an $\eta$ value close to 0 or 1 (peaks in the $\eta$ distribution) are less precise (low resolution region) than reconstructions in the valley of the $\eta$ distribution, where more charge is shared between the channels. Therefore, the resolution is highest at the boundary between strips and lowest in their center.

### 4.3.2 Two-dimensional $\eta$-algorithm

To extract clusters from each sub-frame the photon finding algorithm described previously is used. Each found event consists of the cluster position $(n, m)$ given by the pixel with the highest charge in the cluster and the four charge values sampled at the pixels of the $2 \times 2$ cluster: $Q_{n,m}$, $Q_{n,m+1}$, $Q_{n+1,m}$ and $Q_{n+1,m+1}$. Figure 4.3 shows the 4 adjacent pixels to a cluster and the area spanned between the 4 pixels centers describing the cluster. Similar to the one-dimensional case $\eta_x$ and $\eta_y$ are calculated for the $x$ and $y$ direction:

$$Q_{\text{tot}} = Q_{n,m} + Q_{n,m+1} + Q_{n+1,m} + Q_{n+1,m+1},$$

$$\eta_x = \frac{Q_{n+1,m} + Q_{n+1,m+1}}{Q_{\text{tot}}},$$

$$\eta_y = \frac{Q_{n,m+1} + Q_{n+1,m+1}}{Q_{\text{tot}}}. \hspace{1cm} (4.5)$$

Similar to the one-dimensional case, the parameters $\eta_x$ and $\eta_y$ are non-linear functions of the charge and therefore need to be corrected. A simple separate correction for $\eta_x$ and $\eta_y$ equivalent to the one-dimensional method proved to be not sufficient, since it introduced artifacts in the images originating from the strong correlation of $\eta_x$ and $\eta_y$. Therefore an algorithm considering both parameters simultaneously was developed. In this algorithm the $\eta$-space is sub-divided into $N \times N$ bins, denoted $H_{(x,y)}$. Each bin is associated to a sub-pixel $\Pi_{(x,y)}$ centered in $(\pi_x, \pi_y)$.
Figure 4.2: One-dimensional normalized $\eta$-distribution acquired with a uniform 20 keV photon beam. The two peaks close to $\eta = 0$ and $\eta = 1$ originate from the two strip centers, where little charge is shared with the neighboring pixels.
\[ Q_{\text{tot}} = Q_{n,m} + Q_{n,m+1} + Q_{n+1,m} + Q_{n+1,m+1} \]
\[ Q_R = Q_{n+1,m} + Q_{n+1,m+1} \]
\[ Q_T = Q_{n,m+1} + Q_{n+1,m+1} \]
\[ \eta_x = \frac{Q_R}{Q_{\text{tot}}} \]
\[ \eta_y = \frac{Q_T}{Q_{\text{tot}}} \]

\[(\eta_x, \eta_y) \xrightarrow{\text{cmap}} (\pi_x, \pi_y)\]

Figure 4.3: The left side shows a sketch of the cluster (gray shaded area) at position \((n, m)\) that spans between the 4 neighboring pixel (indicated in black) centers. The area of the cluster is the same as one physical pixel of the detector. On the right side the calculations from the four pixel charge values \((Q_{n,m} \text{ to } Q_{n+1,m+1})\) to the in-cluster position \((\pi_x \text{ and } \pi_y)\) are shown.

in the position space (i.e. the cluster area spanning from the centers of 4 pixels). While the position and the shape of the sub-pixels in the position space are fixed and given by the size of the cluster and \(N\), the size and position of the bins \(H(x,y)\) are adapted by the algorithm in an iterative minimization process.

The input of the minimization process is a set of photon absorption events from a flat illumination, extracted by the cluster finding algorithm. For each event, the parameters \((\eta_x, \eta_y)\) are determined first. After that, the matching bin in the \(\eta\)-space is determined and the intensity count of the corresponding sub-pixel is incremented. Once all events are distributed, the intensity counts of the sub-pixels are compared and the size and shape of all bins \(H(x,y)\) are adapted to attempt to equalize the intensity of all sub-pixels in the next iteration. This process, of assigning the events and adapting the shape of the bins, is repeated until it converges, i.e. the intensities are equal up to some statistical limit, without further adapting the bins shape and size. The counts of all sub-pixels can not be equalized perfectly with a finite set of photon absorption events. The reason for that is, that the distribution of the photon absorption events on the detector surface is a Poissonian process. Therefore, the distribution has a variance given by physics. The set of corner positions of the bins ranging from \(C_{(0,0)}\) up to \(C_{(N+1,N+1)}\) (see figure 4.5) are denoted \(\text{cmap}\), and are used to map \((\eta_x, \eta_y) \in H(x,y)\) to a sub-pixel \(\Pi(x,y)\) while reconstructing an image in a second step. Figure 4.4 shows a black grid representing the borders of \(25 \times 25\) bins after convergence, i.e. after the intensity is equalized in all bins. The histogram in the background (in color scale) represents the density of the photon absorption events in the \(\eta\)-space for an experimentally acquired flat illumination data set. Note that, bins in areas with high photon density are smaller than bins in low photon density areas.

The \(\eta\)-space is fully covered by the bins. Therefore if a bin is changed in shape and size to fulfill the count intensity requirement the adjacent bins will change as well. To express this behavior mathematically the bin is described by the corners (denoted \(C_{x,y}, C_{x,y+1}, C_{x+1,y} \text{ and } C_{x+1,y+1}\) for bin \(H(x,y)\)), that are also shared with neighboring pixels. Changing the distance between two corners (i.e. the edge lengths) will affect the resulting size of the bins sharing the two corners and therefore the collected counts of these bins. To better control the size of a bin with the
Figure 4.4: Visualization of the $\eta$-space for experimental data of the MÔNCH detector. The color coding represents the photon density. The four spots with high density (red spots) are photons collected close to one of the four collecting anodes. The grid rendered on top shows the boundaries of $25 \times 25$ $H_{(x,y)}$ bins after convergence. The size of the bins is smaller in high density regions and lower in low density regions. This ensures a uniform illumination of all sub-pixels.
associated edge lengths and to have a numerical more stable system, each bin is further divided into 4 triangles, each spanning from the bin center point $Z_{x,y}$ to two corners. The edges shared with neighboring bins are denoted $a_{x,y}$, $a_{x,y+1}$ (horizontal) and $b_{x,y}$, $b_{x+1,y}$ (vertical). The bin internal edges dividing the four triangles are denoted $e_{x,y}$, $f_{x,y}$, $g_{x,y}$ and $h_{x,y}$. Note that the corner and center positions are two-dimensional variables. See figure 4.5 for an overview of the variable declaration.

Figure 4.5: The left side shows the variable declaration of one bin $H_{(x,y)}$ in $\eta$-space. The four corners ($C_{x,y}$, $C_{x+1,y}$, $C_{x+1,y+1}$ and $C_{x,y+1}$) span the surface of the rectangular bin. Each bin is further divided into 4 triangles, where $Z_{x,y}$ is the joint corner of these triangles. Each rectangular bin has two vertical (denoted $b_{x,y}$ and $b_{x+1,y}$) and two horizontal (denoted $a_{x,y}$ and $a_{x,y+1}$) edges connecting the corners. Additionally, the triangle edges from the center point $Z_{x,y}$ are named $e_{x,y}$, $f_{x,y}$, $g_{x,y}$ and $h_{x,y}$. The right side shows the variable names of the edges connecting the corner positions with adjacent positions. Note that the corners and edges of a bin are shared with adjacent bins, to assure full coverage of the $\eta$-space.

The area of the gray shaded triangle in figure 4.5 with side lengths $a$, $e$ and $f$ (bin indices dropped for simplicity) is given by Heron’s formula:

\[
A = \sqrt{s(s-a)(s-e)(s-f)}; \\
S = \frac{a + e + f}{2}.
\] (4.6)

The area of the other three triangles completing a bin can be calculated accordingly. The size of the bin is given by the sum of the area of all triangles. The change of the area of a triangle exhibits quadratic growth compared to the edge length. Therefore, if the intensity of a triangle is a factor of $w$ over the desired average level, the length of the edges is multiplied by $1/\sqrt{w}$.

Having established the relationship between intensity counts and edge length, it is now necessary to find a configuration of corner and center positions ($C_{x,y}$ and $Z_{x,y}$) that satisfy the previously calculated new edge lengths. To do this, a relationship of each corner or center point to all neighboring points, where an edge is shared, is set-up. This is done by defining the weighted average
position for the point with the edge length as weight. This results in the following equations for the new corner positions (compare right side of figure 4.5):

\[
C_{x,y} = \frac{1}{8} \left( a_{x-1,y}C_{x-1,y} + b_{x,y-1}C_{x,y-1} + a_{x,y}C_{x+1,y} + b_{x,y-1}C_{x,y-1} +
\right. \\
\left. g_{x,y}Z_{x,y} + h_{x-1,y}Z_{x-1,y} + f_{x-1,y-1}Z_{x-1,y-1} + e_{x,y-1}Z_{x,y-1} \right).
\] (4.7)

And similar for the new center positions:

\[
Z_{x,y} = \frac{1}{4} \left( g_{x,y}C_{x,y} + e_{x,y}C_{x,y+1} + h_{x,y}C_{x+1,y} + f_{x,y}C_{x+1,y+1} \right).
\] (4.8)

To make sure that the η-space is covered completely the corners at the boundary of the η-space are fixed and are given by the following set of equations:

\[
C_{0,y} = \left( 0, \frac{y}{N} \right); \quad C_{N,y} = \left( 1, \frac{y}{N} \right);
\]
\[
C_{x,0} = \left( \frac{x}{N}, 0 \right); \quad C_{x,N} = \left( \frac{x}{N}, 1 \right);
\] (4.9)

Similar to the one-dimensional method the boundaries of the bin grid in practice slightly extends over the range of \((\eta_x = 0, \eta_y = 0)\) to \((\eta_x = 1, \eta_y = 1)\), since the pixel charge reading \(Q_{n,m}\) might be negative after the pedestal subtraction. The set of equation established in equation 4.7, equation 4.8 and equation 4.9 can be solved by a numerical linear equation solver. After that step all the new corner and center positions are available and reassigning the events to the bins can start again. Figure 4.6 shows an overview of the steps done by the algorithm.

### 4.3.3 Analysis of the two-dimensional η-algorithm

The intensity of a bin is defined as:

\[
I_{x,y} = \int_{S_{x,y}} \frac{dI}{d\eta} d\eta',
\] (4.10)

where \(S_{x,y}\) denotes the surface spanned by the four bin corners and \(\frac{dI}{d\eta}\) represents the local count density in the two-dimensional continuous η-space.

To achieve a homogeneous illumination in the final image each sub pixel must have an equal amount of counts. Therefore for each sub-pixel the following condition must be satisfied:

\[
I_{x,y} = \frac{1}{N^2} I \pm \sqrt{\frac{I}{N^2}},
\] (4.11)

where \(I\) represents the total amount of events, \(N^2\) the amount of sub pixels per cluster and \(\sqrt{\frac{I}{N^2}}\) is the error term originating from photon noise. The photon density is distributed according to a Poisson distribution with a mean of \(\mu = I\) and a standard deviation of \(\sigma = \sqrt{I}\). \(\sigma\) can be minimized by increasing the amount of events used for the reconstruction.
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Figure 4.6: This flow chart shows the algorithm to evaluate \( c_{map} \) in an iterative way. If the homogeneous illumination condition is not satisfied, the edge lengths and therefore the virtual pixel alignment is changed and the condition is rechecked.

By assuming the count density is locally constant and \( S_{x,y} \) is only modified in small steps compared to the total surface area, a simplified relationship between the bin area \( A_{x,y} \) (see equation 4.6) and the intensity \( I_{x,y} \) can be established:

\[
I_{x,y} \simeq \frac{dI}{d\eta} A_{x,y}
\]  

(4.12)

The problem the two dimensional \( \eta \)-algorithm tries to solve can be written as a minimization problem of the following form:

\[
\min_{C_{x,y}, Z_{x,y}} \left( I_{x,y} - \frac{I}{N^2} \right)^2 \forall \text{ bins},
\]

(4.13)

where \( \frac{I}{N^2} \) is the desired average intensity of a sub pixel as defined in equation 4.11. By adapting the corner positions \( C_{x,y} \) and the center positions \( Z_{x,y} \) in small steps the algorithm tries to find a minimum. Solving this problem is not trivial since \( I_{x,y} \) is unknown for arbitrary surfaces and the local count density in the \( \eta \)-space (i.e. \( \frac{dI}{d\eta} \)) is unknown. However, one can evaluate \( I_{x,y} \) for
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a given set of $S_{x,y}$ by assigning the events of a flat illumination to the bins. Checking condition equation 4.13 and adapting the triangle corner position allows us to approach a solution in an iterative way (see figure 4.6). Since there are local minima, there is no guarantee that the algorithm will find the overall minimum.

The minimization problem in equation 4.13 only describes how to quantify the residual error, but not how to modify the corner positions. To do this the corner positions are modified according to a simplified linear model. The corner positions are modified by defining criteria for the edge length of the triangles (distance between corners), i.e. edges between triangles with high counts are shorten and edges between triangles with low counts are lengthen for the next iteration. The edge lengths are used to modify the area, and therefore the intensity of the bins.

Because of the relatively low acquisition speed of the current detector system, it is not practical to populate a correction map for each individual cluster. Therefore, small cluster-to-cluster variation like different signal responses of individual pixels are neglected. Future detector assemblies with faster acquisition speeds will allow to maintain a correction map for each individual cluster. To avoid propagation of distortions introduced by dead pixels, a pixel sanity check is performed and events from clusters containing outliers are ignored.

For poly-chromatic sources, where the charge collecting behavior may be energy dependent energy binning might be necessary. This can be achieved by binning the events according to the total charge of an event $Q_{tot}$. This will allow energy dependent imaging and having distinct reconstruction maps for different energy ranges.

4.3.4 Behavior of the two-dimensional $\eta$-algorithm

In this chapter, the behavior of the algorithm with an artificially created data set as input is demonstrated. In figure 4.4 the color coding in the back shows an $\eta$-density distribution for real data acquired with MÖNCH. During a first test phase of the two-dimensional $\eta$-algorithm, it could be observed, that the four peaks in the corner of the $\eta$-space are the most challenging part for the algorithm to cover properly. Therefore, it was decided to test the performance of the algorithm with artificial data with one similar peak at the center of the $\eta$-space. To generate this artificial data set of photons, points are sampled from a two-dimensional Gaussian distribution in $\eta$-space. With a low variance of the Gaussian distribution it is possible to simulate one of the sharp peaks in the corner of figure 4.4. By adapting the variance one could observe the performance for different peak widths. If not other noted, the input of the algorithm are $100 \times 10^3$ points sampled from a two-dimensional Gaussian distribution centered in the middle of the $\eta$-space (i.e. $(\eta_x, \eta_y) = (0.5, 0.5)$). The $\sigma$ for both dimensions is the same and ranges from $10^{-4}$ to 0.1 and can be assumed to be 0.02 if not noted otherwise. Note that, the $\eta$-space covers the pixel pitch area $p^2$. In the case of MÖNCH $p = 25 \mu m$. Therefore, the the variance of the two-dimensional Gaussian distribution can be interpreted as fraction of the pixel size, and has the unit $\mu m$.

In this section, the two-dimensional $\eta$-algorithm is compared to a naive algorithm, called uniform grid. This naive algorithm covers the $\eta$-space between 0 and 1 with a grid of $N \times N$-pixels. All the pixels have the same size and are not adapted in any way to the input. For both algorithms $N$ is always equal.

To quantify the quality of the $\eta$-space coverage, the residual error per triangle is calculated. Given the number of triangles of the coverage, it is possible to calculate the average number of points per triangle. If every triangle contains the average number of points the coverage is ideal. To quantify the quality of the coverage, the difference to that ideal average is calculated for every triangle. The residual error per triangle is then defined as the sum of squared error (i.e. squared
difference to the previously calculated average) per triangle:

\[ \epsilon = \frac{1}{4N^2} \sum_x \sum_y \sum_{\Delta} \left( I_{x,y,\Delta} - \frac{1}{4N^2} I_x I_y \right)^2, \]  

(4.14)

where \( \Delta \) is one of the four triangles in the sub-pixel and \( I_{x,y,\Delta} \) is the intensity count of a triangle.

Figure 4.7a - figure 4.7c show the coverage of the \( \eta \)-space at selected convergence steps for a grid with \( N^2 = 100 \) bins. The horizontal and vertical edges between bins are represented by blue and red lines, respectively. The partitioning of the bins into 4 triangles is represented by green lines. The corner \( C_{x,y} \) of the bins are represented by a green dot. After the first iteration (see figure 4.7a), the convergence shifts in the wrong direction, i.e. the center bins increase their size instead of decreasing. This behavior is independent of the input data set and originates from the initially set edge lengths and the boundary conditions (see equation 4.9). After the first iteration, the coverage steps towards the optimal solution. The triangles in the periphery increase in size, while the size of the center triangles decreases.

Figure 4.7d shows the distribution of the number of counts per triangle for every iteration. The desired mean \( \frac{1}{4N^2} I_x I_y = 250 \), for a total of \( 100 \times 10^3 \) sample points, is indicated by a solid black line. The dashed black lines represent the \( 3\sigma \) boundary. Up to the iteration step 2, the outliers increase their pixel count further, although the overall variance of the distribution decreases continuously, and the mean (indicated by the red line) approaches the desired average continuously.

In figure 4.7e, where the residual error \( \epsilon \) (see equation 4.14) for every convergence step is plotted, it is also visible that the error decreases continuously. For this data set, iteration 22 is the first step where the residual error is higher than in the previous step. Therefore the stop criterion of the algorithm is met in iteration 21, which represents the final coverage for the given input data set.

As previously mentioned, it is most difficult for the algorithm to cover local spikes in the \( \eta \) density distribution. To evaluate the performance of the algorithm different regarding this matter, data sets with peaks with different width are fed to the algorithm. The peaks are represented as two-dimensional Gaussian profiles with different variance. The two-dimensional \( \eta \)-algorithm is run up till convergence, and the residual error is compared to the residual error of a uniform grid coverage with the same amount of bins. Figure 4.8 shows the residual error per triangle for an unconverged \( 10 \times 10 \) grid (i.e. uniform grid) and a converged grid, for different narrow peaks. Below a \( \sigma \) of \( 10^{-3} \) the error for the uniform grid does not increase further, since all sampled points are within one bin cell. At higher variance, the residual error for the uniform grid decreases, since the data set approaches a uniform distribution. The residual error of the \( \eta \)-algorithm decreases linearly with broader peak width, and is in average a factor 3.5 lower than for the uniform grid.

To evaluate the influence of the amount of pixel (i.e. the pixel size) to the residual error another simulation was performed. In this case the standard artificial data set was used but the pixel amount \( N \) was scanned (see figure 4.9). For both algorithm, increasing the pixel size reduced the residual error. In average, the error after running the \( \eta \)-space algorithm is 3 times lower than with a uniform grid.

In summary, the simulations in this section show, that the proposed algorithm performs better on a two dimensional eta distribution with the same amount of bins than the naive uniform grid approach. In all simulations in this chapter, the residual error per triangle is lower for the proposed algorithm under the same test conditions. If the bin count is lower, the number of photons per bin is higher. With the higher photon count per bin, the amount of noise in the reconstructed
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Figure 4.7: Overview of the $\eta\chi$-algorithm. (a), (b) and (c) show the sub-pixel coverage after different iterations. (d) shows the count distribution of the triangles. (e) shows the average quadratic error of all triangles.
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Figure 4.8: Residual error of coverage with $10 \times 10$ virtual pixels for 2d-Gaussian distributions with different variance. For comparison the residual error of a uniform grid (i.e. before the first iteration).

Figure 4.9: Residual error of coverage for 2d-Gaussian distributions with $\sigma = 0.002$ with different amount of virtual pixels starting from $5 \times 5$ up to $40 \times 40$. For comparison the residual error of a uniform grid (i.e. before the first iteration).
position is lower, since the noise contribution of the Poissonian process of the photon absorption is decreased.

4.4 Measurement time limitations

The readout speed of the detector is the major bottleneck of the method at the moment. Currently, acquisition times in the order of hours are needed. With the current frame rate of 1 kHz single photon discrimination is possible up to a photon flux of \( \sim 180 \times 10^3 \) photons mm\(^{-1}\)s\(^{-1}\) (assuming an occupancy of 1/9 hits pixel\(^{-1}\)) [19]. At this count-rate the acquisition of a high-resolution image with 1 \( \mu \)m\(^2\) virtual pixel size and a dynamic range of 8 bit takes \( \sim 1440 \) s. To reduce this acquisition time new read-out electronics with fast network connections are developed by the SLS Detector group at Paul Scherrer Institute. With frame-rates up to 15 kHz the acquisition could be reduced to approximately a minute.

The exposure time is flux-density dependent and is usually in the 10\( \mu \)s range for synchrotron experiments. On the other hand the possible frame rate, given by the read-out electronics is currently a couple of kHz. Therefore, there is a big dead-time, where the detector is busy and insensitive to photons. In future detector developments it is planned to reduce this dead-time as much as possible. Further, with an event driven read-out count rates could be increased significantly. Because of the low occupancy of each sub-frame, complete read-out of the frames from the read-out chip is a significant overhead that could be avoided by identifying absorbed events in the read-out chip and perform a partial read-out.
Chapter 5

X-ray phase contrast imaging

In this chapter, the interaction of x-rays with matter by means of the complex refractive index is discussed. The mathematical description of a wave propagating through a periodic structure is derived. Further on some experimental setups for phase contrast measurements with X-rays at synchrotrons and micro focus X-ray tubes are presented. The grating interferometer is discussed in more detail. Also, improvements to the grating interferometer by simplifying the setup and using MÔNCH and GOTTHARD are shown.

5.1 Electromagnetic wave propagation in matter

From the Maxwell’s equation it can be derived that the electric field of a monochromatic plane wave at a distance $z$ from a point source at time $t$ is:

$$U(z, t) = U_0 e^{i(kz - \omega t)}, \quad (5.1)$$

where $i = \sqrt{-1}$, $U_0$ is a complex vector indicating the amplitude and phase of the electric field at $z = 0$ and $t = 0$, $k = \frac{2\pi}{\lambda}$ is the angular wavenumber in radians per meter. $\lambda$ is the wavelength of the radiation and can be derived from the photon energy $E$ in eV by:

$$\lambda = \frac{hc}{E}, \quad (5.2)$$

where $h$ is the Planck’s constant with $4.1357 \times 10^{-15}$ eV s and $c = 299.79 \times 10^6$ m s$^{-1}$ is the speed of light in vacuum. The angular frequency $\omega = \frac{2\pi c}{\lambda}$ has the units radians per second.

If we are only interested in the change of the initial electromagnetic field $U_0$ at the distance $z$, equation 5.1 can be simplified by ignoring the time factor. Consequently, the time-invariant version of the previous equation is:

$$U(z) = U_0 e^{ikz}, \quad (5.3)$$

This formula is only dependent on the distance to the source point.

Note that it is not possible to measure the electric field $U(z)$ directly. However, it is possible to measure the intensity of the field, which is defined as:

$$I(z) = |U(z)|^2 = |U_0 e^{ikz}|^2. \quad (5.4)$$
Since it is only possible to measure the intensity of the field, which corresponds to the magnitude of \( U(z) \), the information about the phase, which is encoded in the argument of \( U(z) \) is lost while measuring. Therefore, additional techniques are needed to retrieve the phase information of \( U(z) \). Some of these methods are shown in section 5.3.

**Complex refractive index**  In section 2.2 scattering events at the level of individual electrons and atoms are considered. If this is generalized to many atoms with many electrons the math presented previously could become very complex. This can be simplified by restricting ourselves to propagation in the forward direction [82] and looking at the refractive index of a material. Since the described scattering mechanisms involve both, elastic and inelastic processes, the resulting refractive index is a complex quantity, describing the modified velocity of the wave in the material, but also the intensity decay while propagating in the material.

The complex refractive index in the hard x-ray spectrum deviates in small amounts from 1 and is wavelength dependent:

\[
n(\lambda) = 1 - \delta(\lambda) + i\beta(\lambda).
\]  

(5.5)

The real and imaginary part of the deviation can be derived from:

\[
\begin{align*}
\delta(\lambda) &= \frac{n_a r_e \lambda^2}{2\pi f_1^0}; \\
\beta(\lambda) &= \frac{n_a r_e \lambda^2}{2\pi f_2^0},
\end{align*}
\]

(5.6)

where \( n_a \) is the atomic density of the material, \( r_e = 2.8179 \times 10^{-15} \text{ m} \) is the classical electron radius and \( f_1^0 \) and \( f_2^0 \) are energy dependent material properties. These properties were carefully measured by e.g. [83]. Note that \( \delta(\lambda) \) describes the change in the phase velocity and \( \beta(\lambda) \) the change in the amplitude introduced by the material, as explained later in this section.

Figure 5.1 shows \( \delta \) and \( \beta \) parameters for different materials in an energy range of 1 keV up to 30 keV. Note that for low \( Z \) materials, which are common in medical and biological samples, the \( \delta \) (i.e. the phase shift) is much stronger than \( \beta \) (i.e. attenuation). Therefore, recording the phase shift for such samples, increases the extracted information contents. The ratio of \( \frac{\delta}{\beta} \) is in the order of \( 10^3 \) and increases quadratically with the X-ray energy.

The refractive index is the ratio between the propagation speed in the material \( v \) and the free space propagation speed:

\[
n = \frac{c}{v}.
\]

(5.7)

However, it can also be looked at as the ratio between the angular frequency \( \omega \) and the angular wavenumber \( k \):

\[
\frac{\omega}{k} = \frac{c}{n} = \frac{c}{1 - \delta + i\beta}.
\]

(5.8)

If we solve equation 5.8 for \( k \) we have

\[
k = \frac{\omega}{c} (1 - \delta + i\beta);
\]

\[
= \frac{2\pi}{\lambda} (1 - \delta + i\beta).
\]

(5.9)
5.1. ELECTROMAGNETIC WAVE PROPAGATION IN MATTER

Figure 5.1: Complex refractive index for the three elements Carbon, Silicon and Lead. The solid line represents the δ part, the dashed line the β part of the refractive index of the particular element.

The substitution of $k$ into equation 5.1 results in:

$$U(z,t) = U_0 \exp \left[ i \left( \frac{2\pi}{\lambda} (1 - \delta + i\beta) z - \omega t \right) \right];$$

$$= U_0 \exp \left[ i \left( \frac{z}{c} - \omega t \right) \right] \exp \left[ -i \frac{\delta}{\lambda} z \right] \exp \left[ -2\pi \frac{\beta}{\lambda} z \right]. \quad (5.10)$$

The first factor of equation 5.10 represents the phase advance if the wave propagates in vacuum. The second factor is dependent on δ and represents the phase shift introduced by the material and the third factor is the attenuation of the beam by the material and is dependent on β [82].

**Attenuation** The third part of equation 5.10 is the attenuation of a wavefront after traveling through a material of thickness $z$. In section 2.2 equation 2.2 we described the attenuation of the intensity in terms of the mass absorption coefficient. Under consideration of equation 5.4, we can establish the relationship of the β-parameter of the material and the mass absorption coefficient of the material:

$$I_0 \exp (-\mu \rho z) = U_0^2 \exp \left( -2\pi \frac{\beta}{\lambda} z \right)^2;$$

$$\mu = \frac{4\pi \beta}{\lambda \rho}. \quad (5.11)$$

The mass density $\rho$ is related to the atomic density $n_a$ by:

$$\rho = m_an_a, \quad (5.12)$$

where $m_a$ is the atomic mass [82]. Therefore, we can also establish the relation of $\mu$ to the absorptive portion of the atomic scattering factor of a single atom $f_2^0$:

$$\mu = \frac{2r_e\lambda}{m_a} f_2^0. \quad (5.13)$$
The absorption length (or attenuation length) in a material is given by [82]:

\[ l_{abs} = \frac{\lambda}{4\pi\beta} = \frac{1}{2n_a r_e \lambda f_2^0}. \]  

(5.14)

The atomic absorption cross section is also related to the material factor \( f_2^0 \) [82]:

\[ \rho_{abs} = 2r_e \lambda f_2^0. \]  

(5.15)

**Phase shift**  
From equation 5.10 we can conclude, that the phase shift introduced by a material with \( \delta \) and thickness \( \Delta z \) is given by:

\[ \Delta \Phi = \left( \frac{2\pi \delta}{\lambda} \right) \Delta z \]  

(5.16)

This also holds, if the material has different properties and \( \delta \) is dependent on the position. If the beam travels along \( z \) the phase shift in a \( (x, y) \) plane after the sample is given by:

\[ \Delta \Phi(x, y) = \frac{2\pi}{\lambda} \int \delta(x, y, z) dz, \]  

(5.17)

where \( \delta(x, y, z) \) is the position dependent \( \delta \) term.

**Refraction**  
We consider a wedge, with the complex refractive index of \( n = 1 - \delta + i\beta \), where the incident x-rays propagate parallel to the \( z \)-axis and enter the wedge perpendicular to the surface, which is parallel to the \( x \)-axis (see figure 5.2b). Furthermore, the opening angle of the wedge is \( \gamma \). Then, the path length (where the x-rays propagate in the wedge) is given by \( \Delta z = x \tan(\gamma) \) and the phase shift \( \Delta \Phi \) is given by equation 5.16. The wave front has the same phase shift, and therefore the length of the path outside the material has to be equalized at all positions \( dx \). This is only possible if the x-rays are refracted by an angle \( \alpha \):

\[ \sin(\alpha) \ dx = \frac{\lambda}{2\pi} d\Phi. \]  

(5.18)

By using the small angle approximation, the wavefront after the wedge propagates at the angle \( \alpha \):

\[ \alpha \approx \frac{\lambda}{2\pi} \frac{d\Phi(x)}{dx} = \delta \gamma. \]  

(5.19)

Note that in the hard x-ray range \( \delta \) is usually small, and therefore the refraction angles are in the order of \( \mu rad \).

To illustrate these effects on the wave field figure 5.2a shows an example with vacuum and two different materials. An initial wave field \( U \) has the same intensity and phase in all three cases. If the wave field travels in vacuum, the intensity and phase do not change, i.e. \( |U| = |U_0| \). Material \( M_1 \) (center) is a material that introduces a strong phase shift, but has weak absorption. Therefore, \( |U_1| \) is close to \( |U| \), whereas the phase shift \( \Delta \Phi_1 \) is big. On the other hand, \( M_2 \) has low \( \delta_2 \) and a high \( \beta_2 \), and is therefore strongly absorbing. This results in a small \( \Delta \Phi_2 \) and a high difference in the magnitude of \( |U| \) and \( |U_2| \). Note that the depth of the two materials is also different. Also note that the wave length is not in scale with the \( z \) axis.
Figure 5.2: (a) An initial equal (same intensity and phase) wave field $U$ travels in vacuum, and two different materials $M_1$ and $M_2$. $M_1$ introduces a strong phase shift and weak absorption, whereas $M_2$ is strongly absorbing. (b) A coherent beam traverses a wedge with angle $\gamma$. After the wedge the beam travels at an angle $\alpha$.

5.2 Huygens-Fresnel principle

Considering an aperture $\Sigma$ in the $(\xi, \eta)$ plane illuminated from the negative $z$ direction, the wave field at the $(x, y)$ plane can be calculated with the Huygens-Fresnel principle (see figure 5.3). For a point $P_0$ in the $(x, y)$ plane the wave field is given by:

$$U(P_0) = \frac{1}{i\lambda} \int \int_{\Sigma} U(P_1) \frac{\exp(ikr)}{r} \cos \theta \, ds,$$

(5.20)

where $P_1$ is the known wave field at a point in the $(\xi, \eta)$ plane, $\theta$ is the angle between the $z$-axis and the vector connecting $P_0$ and $P_1$ and $r$ is the distance between $P_0$ and $P_1$ [84]. Furthermore, $ds$ is the infinitesimal of the area $\Sigma$.

Since $\cos \theta = \frac{z}{r}$ equation 5.20 can be rewritten as:

$$U(x, y) = \frac{z}{i\lambda} \int \int_{\Sigma} U(\xi, \eta) \frac{\exp(ikr)}{r^2} \, d\xi \, d\eta.$$

(5.21)

The distance $r$ between $P_0$ and $P_1$ is given by:

$$r = \sqrt{z^2 + (x - \xi)^2 + (y - \eta)^2}.$$

(5.22)

**Fresnel approximation** The main problem for solving the above-mentioned integral is the expression of $r$. With the Fresnel approximation $r$ can be approximated, since the Taylor expansion of $\sqrt{1 + b}$ is given by:

$$\sqrt{1 + b} = 1 + \frac{1}{2} b - \frac{1}{8} b^2 + \ldots,$$

(5.23)
Figure 5.3: Huygens-Fresnel principle: variable declaration [84].

and equation 5.24 can be expressed as:

$$r = z \sqrt{1 + \left(\frac{x - \xi}{z}\right)^2 + \left(\frac{y - \eta}{z}\right)^2},$$

(5.24)

we can approximate $r$, by only keeping the first terms of the expansion, with:

$$r \approx z \left(1 + \frac{1}{2} \left(\frac{x - \xi}{z}\right)^2 + \frac{1}{2} \left(\frac{y - \eta}{z}\right)^2\right).$$

(5.25)

The distance $r$ appears twice in equation 5.21. For the denominator, the error introduced by dropping all terms but $z$ is generally small an acceptable. Whereas, the $r$ appearing in the exponent has a big influence on the phase, since it is multiplied by the angular wave number, which is small in the case of hard x-rays. Therefore, $r$ in the exponent is replaced by all terms of equation 5.25. This results in the Fresnel diffraction integral [84]:

$$U(x, y) = e^{ikz} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} U(\xi, \eta) \exp \left[\frac{ik}{2z} ((x - \xi)^2 + (y - \eta)^2)\right] d\xi d\eta.$$  

(5.26)

Transfer function based Fresnel propagation  Equation 5.26 can be interpreted as a two-dimensional convolution of the form:

$$U(x, y) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} U(\xi, \eta) h(x - \xi, y - \eta) d\xi d\eta;$$  

(5.27)

where $*$ is the convolution operator and

$$h(x, y) = \frac{e^{ikz}}{i\lambda z} \exp \left[\frac{ik}{2z} (x^2 + y^2)\right].$$  

(5.28)

Since the convolution theorem states that a convolution can be replaced by the multiplication of the Fourier transformed arguments, equation 5.27 can be rewritten:

$$U(x, y) = \mathcal{F}^{-1} \{\mathcal{F} \{U\} \mathcal{F} \{h\}\}.$$  

(5.29)
The Fourier transform of equation 5.28 is given by \[84\]:

\[
H(f_X, f_Y) = \mathcal{F}\{h\} = e^{ikz} \exp \left[ -i\pi\lambda z(f_X^2 + f_Y^2) \right],
\]

(5.30)

where \(f_X\) and \(f_Y\) are the signal intensities and phases of the spatial frequency \(f\) in \(x\) and \(y\) direction, respectively.

The concept explained in this section is revisited in section 5.4.2, where the Talbot effect is explained. In particular, the transfer based Fresnel propagation is used to evaluate the wave field downstream a periodic structure.

### 5.3 Methods

This chapter gives a brief overview of phase imaging methods, used in the hard x-ray regime. \[85\] gives a more complete overview over the different methods and also discusses the requirements in more detail.

---

**Crystal interferometer**  Beam splitting interferometer, such as the Mach-Zehnder interferometer, are common in visible light interferometry. The first implementation for the hard X-ray energy range was the Bonse-Hart Interferometer in 1965 \[23\]. The coherent X-ray beam is split by a silicon crystal before the sample (see figure 5.4a). While one part of the beam passes the sample it experiences a phase shift. Three more Si crystals are necessary to recombine the unchanged beam with the beam altered by the sample. Interference between the two beam generates intensity modulations proportional to the phase shift introduced by the sample. This intensity modulations are detectable by a conventional X-ray detectors.
CHAPTER 5. X-RAY PHASE CONTRAST IMAGING

One major limitation of the crystal interferometer is the mechanical stability. The length difference of the two paths needs to be well below the wavelength of the light (i.e. below one nanometer for hard X-rays). Therefore, the four beam splitters are usually on one single crystal, while its size limits the sample size. It also limits the photon energy, since the diffraction angle decreases with higher energies, and therefore full separation of the beam requires larger propagation distances. Additionally, a high photon flux is needed, because of the low efficiency of the crystals, thus making this interferometer unpractical for X-ray tube setups.

**Analyzer based imaging** or Diffraction enhanced Imaging (DEI), first mentioned by Chapman et al. [86], works by selectively observing only radiation which is refracted by a certain angle in the sample. This is achieved by having an analyzer crystal after the sample in the monochromatic synchrotron beam (see figure 5.4b). The analyzer is tilted or rocked in small steps and the rocking curve is recorded. While rocking the analyzer, differently refracted parts of the beam are forwarded to the detector, since they have a different angle as explained in equation 5.19. The shift of the peak of the rocking curve indicates the phase shift introduced by the sample. The concept has also been extended to two-dimensional phase gradient detection [87]. It is also possible to perform tomography with this setup. A density resolution of 1 mg/cm$^3$ has been reported [88, 89].

**Propagation based imaging** allows a simple setup. It relies on the fact that the source of the beam provided by third generation synchrotrons is small (i.e. in the order of 100 µm) and at large distances (up to ~ 50 m) from the experiment table. In this configuration, a point like coherent source and a nearly parallel beam can be assumed. It can be shown that, if the parallel beam impinges the sample-air interface at a slope, that the wavefront will be deflected. Rough estimation for photon energies between 10 keV and 50 keV show, that the angle of deflection is in the order of $10^{-5}$ to $10^{-6}$ radians. This results in a 5 to 10 µm displacement of the beam at a distance of 1 m between the sample and the detector [24]. It is possible to measure quantitative phase information of a sample by acquiring images at different sample to detector distances (as indicated in figure 5.4c). This simple setup, with no additional optical elements, allows high spatial resolution imaging, that is only limited by the source size and the detector resolution. However, the reconstruction of the phase is not straightforward and often leads to artifacts. Propagation based imaging with hard x-rays was first shown on a synchrotron by [24], and later on also with a micro focal tube source by [90].

**Grating interferometry**, as shown in figure 5.4d, is a more recently demonstrated approach to measure the refraction angle of hard X-rays introduced by the sample [91, 39]. The main optical component of a grating interferometer is a binary phase grating $G_1$, that refracts the incident radiation. The diffraction angle is very small and in the order of $\mu$rad. The sample introduces distortions to the interference pattern, that are related to the phase shift introduced by the sample. It has been shown that very small refraction angles, in the order of 10 $nrad$, can be detected and the method can also be used for tomographic imaging with a density resolution in the order of 0.5 mg/cm$^3$ [92]. The method is explained in more detail in section 5.4.
5.4 Grating interferometry

5.4.1 Working principle

Figure 5.5 shows a sketch of a grating interferometer. A fully coherent monochromatic wave field is incident to a transmission grating $G_1$ of period $g_1$. A part of the wave field is diffracted into the first diffraction orders, which propagate at a small angle, given by $\lambda/g_1$. The positive and negative diffracted waves interfere downstream of the grating, and generate a periodic intensity modulation at a distance $D$. The condition so that an intensity modulation appears are discussed in section 5.4.2. If a sample is introduced in the fully coherent wave field, it will introduce phase changes to the planar wave field. These phase changes will alter the intensity pattern at distance $D$. By recording the pattern with and without sample, it is possible to deduce the phase shift introduced by the sample, by comparing the two recorded signals.

Typically, the distance between the interference fringes produced at a distance $D$ is smaller than the spatial resolution of the detector. Therefore, an absorption grating (denoted $G_2$) is placed in front of the detector. The period $g_2$ of $G_2$ is chosen, such that it is equal to the intensity pattern period of the interference fringes. $G_2$ is then stepped in front of the detector and for each step the image is recorded. In this way the position and shift of the interference fringes can be determined although the detector does not have the required resolution.

To relax the constraint of the fully coherent source [27] suggest using a third grating, denoted $G_0$, directly after the x-ray source. $G_0$, typically is an absorbing mask with transmitting
slits, creates an array of individually coherent, but mutually incoherent sources, and thus enables
the use of low-brilliance X-rays sources like XRTs for phase contrast imaging.

5.4.2 Talbot effect

In 1836 Henry Fox Talbot first observed [93], that if an object with a periodic structure is illu-
minated with plane waves, the image of the periodic structure is repeated at regular distances
to the object plane. The Talbot length, where the first (self) image occurs is denoted \( z_T \), and
further self-images occur at distances \( m z_T \), where \( m \in \mathbb{N} \). Furthermore, at half the Talbot length
a phase-shifted self image occurs, and at a quarter of the Talbot length, the self image with half
the size occurs (see figure 5.6a).

The Talbot-effect can be shown, by representing the transfer function \( t(\xi) \) of the one-dimensional
periodic structure (i.e. the grating) by a Fourier series:

\[
t(\xi) = \sum_{n=-\infty}^{\infty} a_n \exp \left( 2\pi i \frac{n}{d} \xi \right),
\]

where \( a_n \) is the \( n \)th Fourier coefficient, with \( n \in \mathbb{N} \), and \( d \) is the period of the structure [94].
Note that the Fourier series can represent an array of slits, absorption gratings, phase gratings
or any other periodic structure with a period of \( d \). This is possible by choosing the Fourier
coefficients \( a_n \) appropriately. The Fourier coefficients become complex, if the transfer function
describes a structure that introduces a phase shift to the propagating wave field.

It is assumed, that the structure is illuminated by a unit-amplitude, normally incident plane
wave. Therefore, the field immediately after the structure is equal to the transfer function: \( U(\xi) = t(\xi) \).
One way to evaluate the wave field at any distance \( z \) from the grating, would be by using the
integral shown equation 5.26. A simpler approach is, to take the Fourier transform of \( U(\xi) \) and
multiply it by the Fourier transform of the Fresnel propagator (see equation 5.30) and taking the
inverse Fourier transform. This method is described previously by equation 5.29.

The Fourier transform of a Fourier series, and therefore of \( U(\xi) \), is given by:

\[
\mathcal{F} \{ U(\xi) \} = \sum_{n=-\infty}^{\infty} a_n \delta \left( f_X - \frac{n}{d} \right),
\]

with \( \delta(a) \) being the Dirac delta function. The Fourier transform of the propagator (see equa-
tion 5.30) can be simplified to one dimension, and the constant term \( \exp(ikz) \) can be omitted:

\[
H( f_X ) = \exp \left( -i \pi \lambda z f_X^2 \right).
\]

Now, we can describe the Fourier transformed wave field at distance \( z \):

\[
\mathcal{F} \{ U(x) \} = \sum_{n=-\infty}^{\infty} a_n \delta \left( f_X - \frac{n}{d} \right) \exp \left( -i \pi \lambda z f_X^2 \right).
\]

By investigating equation 5.32, we can see that equation 5.34 yields non-zero results only, if \( f_X = \frac{n}{d} \).
Therefore, it is sufficient to evaluate \( H(f_X) \) only at frequencies where \( f_X = \frac{n}{d} \):

\[
H \left( f_X = \frac{n}{d} \right) = \exp \left( -i \pi \lambda z \frac{n^2}{d^2} \right).
\]
Inverse transforming the spectrum given by equation 5.34 yields the field at the distance $z$ from the grating:

$$U(x) = \int_{-\infty}^{\infty} \left[ \sum_{n=-\infty}^{\infty} a_n \delta \left( f x - \frac{n d}{2} \right) \exp \left( -i\pi\lambda z \frac{n^2}{d^2} \right) \exp \left( i2\pi f x \right) \right] df x$$

$$= \sum_{n=-\infty}^{\infty} a_n \exp \left( -i\pi\lambda z \frac{n^2}{d^2} \right) \exp \left( i2\pi \frac{n}{d} x \right).$$

(5.36)

Note that if $z = md^2/\lambda$, with $m$ an even integer, the first exponential term vanishes and equation 5.36 simplifies to the transfer function of the grating (see equation 5.31) [95]. If $m$ is odd, this term becomes $-1$ and the self-image of the grating is shifted by $d/2$. The Talbot distance $z_T$ is where the first self image occurs:

$$z_T = \frac{2d^2}{\lambda}.$$  (5.37)

Figure 5.6 shows simulations of the intensity of Talbot carpets for different grating structures. The beam has an energy of 17.6 keV and is parallel to the $z$ axis. The repetition period $d$ is 4.7 $\mu m$ for all simulations. For Figure 5.6a and Figure 5.6b the transfer function is real (i.e. absorption only, no phase shift), and the self-images appear at a distance $z_T$ from the grating. Also, at fractions of the Talbot distance smaller or shifted self-images occur. Since, it is only possible to detect the intensity, phase shifting structures have either no visible self image (see figure 5.6c) or the distance is shifted. For the $\pi/2$ phase shift grating in figure 5.6d, the highest intensity oscillation appears at $z_T/4$. For all phase contrast experiments in this thesis a $\pi/2$ phase grating was used, and therefore the distance from $G_1$ to the detector was $\approx 16 \text{ cm}$.

5.5 $G_2$-less grating interferometry

Using $G_2$ in the grating interferometer, decouples the sensitivity of the instrument from the detector resolution. However, it comes at the price of a lower dose efficiency, since $G_2$ is usually an absorption grating with 50% duty cycle, and it therefore absorbs half of the photons. Phase stepping also introduces extra mechanical complexity to the system, since the stepping procedure requires fine steps below the pixel size of the detector. Additionally, the scanning time is increased. Finally, a strict set of requirements concerning $G_2$ renders the manufacturing challenging. Specifically, the large imaging field of views (hundreds of square centimeters) required by medical applications, which means that dense micro structures have to be produced over a large area with a high uniformity in terms of depth, duty cycle, and period [96]. $G_2$-less grating interferometry overcomes many of the mentioned limitations and has the potential to increase the acceptance of phase contrast imaging, specifically for medical applications.

The $G_2$-less grating interferometer used in this thesis consists of two components. The grating, which was manufactured in-house at PSI. It is a one-dimensional $\pi/2$ grating with a duty-cycle of 50% and a pitch of 4.7 $\mu m$, edged in a silicon substrate. The field-of-view of the grating is roughly 2 cm $\times$ 2 cm, and exceeds the size of the field-of-view of the detector. To have a $\pi/2$ phase shift at the design energy of 17.6 keV the grooves are edged $\approx 30 \mu m$ deep. The second component is the silicon hybrid semiconductor detector placed at a distance of $\approx 16 \text{ cm}$, which is one fourth of the Talbot distance of the grating. The working principle of such detectors are explained in chapter 3.
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Figure 5.6: Calculated interferograms for different slit and grating patterns illuminated by a perfect coherent source. The beam has an energy of 17.6 keV and the period of the structure is 4.7 µm.
5.6. PHASE RETRIEVAL METHODS

While omitting \( G_2 \) relaxes many constraints on the setup, it increases the requirements for the detector. One major requirement is that the detector must be capable of resolving the fringe pattern without the help of an absorption grating. Therefore, the detector needs a better position resolution than the fringe image of 4.7 \( \mu m \). With the silicon hybrid detectors and the help of single photon interpolation algorithms used in this thesis, this requirement was just met, and the pattern could be resolved.

5.6 Phase retrieval methods

Phase retrieval is the process of comparing two signal acquired with the grating interferometer. Usually, a first measurement, where the fringes of the phase grating are recorded, is compared to a second measurement, where the sample and the phase grating are in the beam. By comparing the two signals, the phase shift introduced by the sample can be extracted. In this thesis the standard grating (with a period of 4.7 \( \mu m \)) used with \( G_2 \), was also used for the measurement without \( G_2 \). This small period is not well matched to the resolution of the detector using interpolation and currently the fringes can only be resolved at the boundaries between pixels. Therefore, the recorded signals of a grating interferometer with and without \( G_2 \) are currently quite different (explained in the next sub-section). In the future phase gratings with larger pitches will be used, allowing to resolve the interference fringes everywhere in the pixel. Then the signals for the two methods are very similar. Three different methods for the phase retrieval are presented here. The first is preferred for the conventional grating interferometer, the others yield better results in the case of a \( G_2 \)-less setup. Another popular method is the moiré-fringe method shown in [95].

5.6.1 Acquisition protocols

If a \( G_2 \) is stepped in front of the detector, the step size and the number of steps is chosen, such that one period of the fringe pattern is recorded. For each pixel a phase-stepping curve (PSC) is generated for the reference and the object measurement, as depicted in figure 5.8 [39]. If the PSC contains exactly one period of the fringe, the absorption, phase and scattering signal are encoded in the phase and magnitude of the first and second coefficient of the Fourier transformed PSC (see section 5.6.2 for more details).

Due to the too low resolution (compared to the period) in the pixel center, the single-photon based position interpolation algorithms presented in chapter 4 provide a less clean signal, than the PSC. Figure 5.7 shows a reference and object fringe measurement for one channel couple (two half channels) of the GOTTHARD detector. The couple is sub-divided into 64 virtual channels, by the interpolation algorithm (see section 4.1). The high amplitude oscillation to the right of the center (around virtual channel 20) represents the recorded fringe from a phase grating with a pitch of 4.7 \( \mu m \). The signal is only present, where the charge sharing effect (see section 3.3) between the two channels of the couple is most pronounced, and therefore a high spatial resolution is achieved. The region with the high spatial region should be in the center of the channel couple. However, it is shifted closer to the left channel, since the read-out electronics introduces some distortion to the pixel signals. These issues are the main reason that more sophisticated phase retrieval methods are required for this signal, than for the PSC of a conventional grating interferometer.
Figure 5.7: Fringe pattern of a $G_1$ with 4.7 $\mu$m pitch, acquired with the $G_2$-less grating interferometer using GOTTHARD. This is the signal after the position interpolation. The channel couple of two 25 $\mu$m channels are sub-divided into 64 virtual channels. Two measurements are shown. One with (red line) and one without (blue line) sample.

5.6.2 Fourier transform based method

Figure 5.8 shows a possible PSC acquired without a sample (reference scan) and with a sample (object scan). The data-points indicate the steps of the stepping procedure of $G_2$. The stepping distance is so that one complete fringe period is recorded in $n = 16$ steps. To extract the two contrasts, namely absorption ($A$) and differential phase shift ($\Delta \varphi$), the reference and object signal are Fourier transformed, yielding $n$ complex Fourier coefficients, denoted $c_i$. The magnitude of $c_i$ is denoted, $a_{i,\text{ref}}$ or $a_{i,\text{obj}}$, respectively. The phase of the complex coefficient $c_i$ is denoted, $\varphi_{i,\text{ref}}$ or $\varphi_{i,\text{obj}}$, respectively. The two contrasts are encoded in the first and second coefficients of the two signals:

$$A = 1 - \frac{a_{0,\text{obj}}}{a_{0,\text{ref}}},$$
$$\Delta \varphi = \varphi_{1,\text{obj}} - \varphi_{1,\text{ref}}.$$  \hspace{1cm} (5.38)

The absorption signal $A$ corresponds to the reduction of the mean intensity of the PSC and $\Delta \varphi$ to its shift. The absorption signal $A$ is equal to the absorption signal retrieved by conventional absorption imaging without a grating interferometer.

The grating interferometer allows to extract an additional contrast named scattering contrast (denoted $V$). Although, not extensively investigated in this thesis, it is mentioned here for completeness. The scattering signal represents the high spatial frequency phase shift introduced by a sample. I.e. if the differential phase shift has a lower spatial frequency than the grating period, it is visible in the differential phase shift signal. If the frequency is higher it contributes to the scattering contrast. The scattering contrast can be extracted from the PSC with:

$$V = \frac{a_{1,\text{obj}} a_{0,\text{ref}}}{a_{0,\text{obj}} a_{1,\text{ref}}}. \hspace{1cm} (5.39)$$

$V$ represents the reduction of the amplitude of the PSC introduced by the sample.
5.6. PHASE RETRIEVAL METHODS

Figure 5.8: Simulated phase shift curve (PSC) from a conventional grating interferometer.

5.6.3 Hilbert transform based method

To account for the mismatch of the detector resolution and the grating period $p$ (see figure 5.7), a new method of phase retrieval was developed. For GOTTHARD, one absorption and one differential phase shift signal is extracted per channel couple. In the case of MÖNCH one absorption and one differential phase shift signal is extracted per cluster. This means, that the resulting images have a pixel size of 25 $\mu m^2$ for MÖNCH and 25 $\times$ s $\mu m^2$ for GOTTHARD, where $s$ is the step size parallel to the grating lines. To improve the SNR for the pixelated detector, the intensities of the virtual pixels are integrated for one cluster along the grating lines. Therefore, two one-dimensional signals (i.e. reference and object signal) are available per pixel cluster.

The recorded interference fringe can be approximated by a sinusoidal signal:

$$ I(x) = a(x) + b(x) \cos \left( \frac{2\pi}{g_1} x - \phi(x) \right), \quad (5.40) $$

where $-p/2 \leq x < p/2$ is the in-cluster or in-channel couple position (virtual pixel or channel), and $p$ is the cluster or channel pitch of the detector [19]. $g_1$ is the period of the recorded interference pattern, $a(x)$ contains the absorption information. $b(x)$ contains the scattering or visibility reduction and the response of the pixel cluster due to non-uniform resolution. $\phi(x)$ is the phase information of the sample [19].

$I_g(x)$ and $I_s(x)$ represent the intensity modulation of the grating (reference) and the sample (object) image, respectively. The absorption signal is extracted by the ratio of the cumulative intensities over a channel couple or cluster:

$$ A = 1 - \int_{-p/2}^{p/2} \frac{I_s(x)}{I_g(x)} \, dx. \quad (5.41) $$

The phase signal $\Delta \phi$ is extracted by generating the analytical signals $\hat{I}_s(x)$ and $\hat{I}_g(x)$ from the
sample or grating signal, respectively:

\[ \Delta \varphi = \int_{-p/2}^{p/2} w(x) \arg \left\{ \frac{\tilde{I}_s(x)}{\tilde{I}_g(x)} \right\} \, dx, \quad (5.42) \]

where \( w(x) \) is a weighting function, which accounts for the non-uniform resolution of the interpolation method. It is chosen, such that in regions where the resolution is low (i.e. channel or pixel centers), the weight is low, and vice versa. In most cases, a Gaussian distribution was chosen for \( w(x) \). Note, that the weighting of the intensity reduces the dose-efficiency of the reconstruction method, since photons in the center are effectively discarded.

The analytical signal \( \tilde{I}(x) \) is defined as \( I(x) \) without the negative frequency components. This can be achieved by performing the Hilbert transform on \( I(x) \) and add the Hilbert transformed signal to the original signal:

\[ \tilde{I}(x) = I(x) + i\mathcal{H}\{I\}(x), \quad (5.43) \]

where \( \mathcal{H} \) is the Hilbert transform and is defined as:

\[ \mathcal{H}\{I\}(x) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{I(\tau)}{x - \tau} \, d\tau. \quad (5.44) \]

\( \mathcal{H}\{I\}(x) \) has the effect of shifting the phase of the negative frequency components of \( I(x) \) by \( +90^\circ \left( \pi/2 \text{ radians} \right) \) and the phase of the positive frequency components by \( -90^\circ \). Furthermore, \( i\mathcal{H}\{f\}(y) \) has the effect of restoring the positive frequency components while shifting the negative frequency ones an additional \( +90^\circ \), resulting in their negation.

The resulting analytical signal is a complex signal, that encodes the instantaneous phase of the original signal in its argument. Therefore, it is possible to extract the phase shift introduced by the sample, by taking the ratio of the two recorded signals and extract the argument, as shown in equation 5.42.

### 5.6.4 Sinusoidal model based method

With this method, a sinusoidal model is fitted to the acquired signal with a least-square algorithm. As a first step for MÖNCH, the signal of each cluster is projected along the grating lines to have a one-dimensional signal in the same manner as for the Hilbert transform based method. Then for each cluster, the average of the signal is subtracted, so that the absorption term vanishes. The sinusoidal model corresponds to the approximation of the interference fringe, introduced for the Hilbert transform based method (see equation 5.40), multiplied with a Gaussian window. The intensity of the in cluster position \( x \) of the cluster \( c \) can be approximated with:

\[ I^c(x) = \frac{1}{\sigma_w \sqrt{2\pi}} \exp \left\{ -\frac{x^2}{2\sigma_w^2} \right\} G^c \cos \left\{ \frac{2\pi}{g_1} x - \varphi^c \right\}, \quad (5.45) \]

where \( \sigma_w \) is the width of the Gaussian window and \( g_1 \) is the grating period of \( G_1 \). These parameters are common for all clusters of one acquisition. The parameter \( \sigma_w \) is evaluated by scanning a range and comparing the signal-to-noise ratio of the resulting image. The parameter \( b^c \) and \( \varphi^c \) are fitted with the least-square algorithm for each cluster. \( b^c \) encodes the fringe visibility and \( \varphi^c \) the phase.
Figure 5.9: Sinusoidal model for fitting the phase signal of a $G_2$-less grating interferometer. The data points of the two measurements are fitted with a cosine multiplied by a Gaussian window, therefore only the data points in the center of a cluster contribute to the phase signal.

By repeating the least-square fit for the grating fringe $I_g^c(x)$ and the sample fringe $I_s^c(x)$, it is possible to extract the differential phase shift by:

$$\Delta \varphi^c = \varphi_g^c - \varphi_s^c. \quad (5.46)$$

Figure 5.9 shows the grating (in red) and sample fringe (in blue) of a random cluster fitted with the sinusoidal model. The width of the Gaussian window is selected, so that only the high resolution region of the cluster contributes to the fit. The width is evaluated by scanning a range, as shown in section 8.2. Inside the window, the data points are fitted with a cosine function. For this example cluster, $\Delta \varphi^c$ is $-1.15$ rad. The sample reduced the amplitude by 25%.
Chapter 6
Detector Characterization

In this chapter experiments, that are done to characterize the MÔNCH detector, are shown. In section 6.1 the energy calibration of the detector under consideration of the charge sharing effect is demonstrated. The model used to fit the spectra was previously published in [77], and the experimental results for MÔNCH are also previously published in [19]. Section 6.2 discusses noise measurements for MÔNCH, while section 6.3 is a quick demonstration of the cluster finding algorithm (described in section 4.2) with experimental data. In section 6.4 an experiment to explore the charge sharing effect in dependency of the absorption depth in the sensor is described. The results shown in this section are partly also published in [53]. In section 6.5 an experiment to measure the spatial resolution is presented. All experimental data shown in this chapter is acquired at the Synchrotron Radiation for Medical Physics (SyrmeP) beamline at the Elettra Sincrotrone, Trieste, Italy [97].

6.1 Energy Calibration

In order to determine the photon energy of absorbed photons, a precise gain calibration is necessary. The gain $G$ needs to be determined for each pixel of the MÔNCH detector. With the gain, the signal pulse height, with unit mV or analog-digital-converter units (ADUs), can be converted into energy or charge. The charge $Q$ produced by the photon absorption is related to the photon energy. For silicon sensors the relation is: $Q = E/3.6 \, \text{eV}$, where $E$ is the photon energy.

The spectra of a single MÔNCH pixel at different energies are shown in figure 6.1. The spectral fit with the model presented in section 3.3 is indicated by the solid line. It has been shown that the parameter $\alpha$ for all pixels of the first supercolumn of MÔNCH is $82.6 \pm 0.9$ % at 10 keV and $71.8 \pm 0.6$ % at 20 keV [77]. The noise contribution $\sigma$ has been measured to be $170 \pm 18$ eV and $219 \pm 10$ eV for 10 keV and 20 keV, respectively [77]. Note that section 6.2 shows an alternative to measure the noise of a detector. With this method the noise could be reduced further.

Figure 6.2a shows the gain for each pixel of the first supercolumn of MÔNCH. An average value of $G = (100.6 \pm 2.5)$ ADU keV$^{-1}$ has been calculated for the first supercolumn of MÔNCH [19]. The 3 % spread among the pixels is due to manufacturing mismatches, but also to a reduction of the signal amplitude for pixels further away from the readout pads, due-to discharge of the storage capacitors during the readout time (signal droop). In Figure 6.2b the signal droop is shown, by projecting the gain map of figure 6.2a onto the y-axis, which is also the read-out direction. The charge loss during read-out is clearly visible. To evaluate the gain dispersion caused by manufacturing mismatches only, the signal droop is fitted with a linear model:
Figure 6.1: Spectrum of a single MÖNCH pixel at different energies. The solid line shows the fit using equation 3.14. The dashed line shows the Gaussian fit of the pedestal value (dark signal peak) [19].

\[ G(y) = (104.5 - 0.05y \pm 0.9) \text{ ADU keV}^{-1} \]

Under consideration of the signal droop along the y-axis, the pixel-to-pixel variation of the gain be reduced below 1%.

Figure 6.2c shows the gain deviation of the pixels of row y. The later read-out of the storage capacitor at higher pixel rows also causes a small increase in the row gain deviation. It is assumed, that the leakage of the storage capacitor is different for each pixel due to manufacturing mismatches. Therefore, a later read-out will amplify these mismatches more and will cause a higher deviation.

6.2 Noise measurement

A very important parameter for a detector system is its noise, which in the case of MÖNCH is dominated by the electronic noise. The noise determines directly the energy resolution, and since for interpolation the position relation depends on the signal-to-noise ratio (SNR) it also determines the achievable position resolution. One method to determine the noise is to use the charge sharing model described in section 3.3 and consider \( \sigma \) as noise contribution. With the small pixel size of MÖNCH, this renders inaccurate results, since the spectrum is convoluted with partial charge collection from pixel border and corner regions. Therefore, the noise in ADUs is measured directly by fitting the pedestal fluctuations with a Gaussian. The signal pedestal of a detector is the signal if no photons are absorbed. With the gain calibration shown in section 6.1, it is then possible to determine the noise in eV. Furthermore, the noise in eV can be back-calibrated to electrons, corresponding to the equivalent noise charge (ENC) in electrons.

Figure 6.3a shows the noise for each pixel of the first supercolumn of the MÖNCH prototype. The average noise of all pixels is 109 eV (rms) with a fluctuation of \( \pm 7.5 \text{ eV} \) in high gain mode. This corresponds to \( 30 \pm 2\text{e}^\text{−} \text{ENC} \) (rms).
Figure 6.2: (a) Gain map of the first super-column of MÖNCH. Calibrated with a 20 keV beam. (b) projection of the gain onto the y-axis. The error bar represents the standard deviation of the pixel row. The signal droop caused by a delayed read-out is clearly visible. (c) the deviation of the gain per row (i.e. error bar in (b)) has a slight increase if the row is read-out later.
In figure 6.3b spectra of three randomly selected pixels (circled in figure 6.3a) are shown. The dashed line represents the Gaussian fit. The noise of all pixels is represented with the black line.

To investigate the impact of the storage capacitor leakage during read-out, the average noise for each row is plotted in figure 6.3c. The linear fit indicates a small reduction in the noise, if the pixel is read-out later. This can be caused by general signal reduction, and therefore also reduction of the noise.

6.3 Cluster charge

The cluster finding algorithm (CFA) presented in section 4.2 extracts single photon from short acquisitions. This is necessary to analyze the photon absorption events and extract the position as well as the photon energy.

Figure 6.4 shows the raw spectra of all pixels in black, the histogram of the sum of all 4 (9) pixel values of extracted $2 \times 2$ ($3 \times 3$) clusters in red (green). The spectrum of the single pixel contains all pixel values, even if no photon is detected. Hence the peak at 0 keV, caused by detector noise. For the $2 \times 2$ and $3 \times 3$ clusters only photon events are plotted, and therefore there is no increase at the noise peak.

The single pixel spectrum is fitted (solid black line) with the charge sharing model shown in section 6.1, while the $2 \times 2$ and $3 \times 3$ cluster spectra are fitted with a Gaussian (solid green and red line). Note that the width of the peak of the $3 \times 3$ cluster spectrum is bigger than of $2 \times 2$ cluster spectrum, since the noise of more pixel is accumulated.

6.4 Charge sharing study

Parts of this section are a reprint of the publication [53]. Understanding charge sharing as a function of the photon absorption depth and sensor bias is a key for optimal processing of single photon data for high resolution imaging. In this experiment, the charge sharing effect is investigated in detail by looking at single photon events detected with the pixellated MÔNCH detector system at different photon absorption depths in the sensor. The charge sharing is addressed as a function of the absorption depth, as the position resolution is dependent on this parameter [53]. Furthermore, the influence of the electric field strengths on the resulting signal response of the detector is investigated by changing the applied sensor bias voltage.

To control the interaction depth in the sensor, the detector system was edge-on illuminated by a monochromatic beam with 20 keV photon energy at the Synchrotron Radiation for Medical Physics (SYRMEP) beamline at the Elettra Sincrotrone, Trieste, Italy [97]. The beam was collimated by a 5 $\mu$m wide Tungsten slit (see figure 6.5). With the X-ray source at 23 m distance and a slit-to-detector distance of 10 cm, a nearly ideal box-illumination of 5 $\mu$m height can be assumed. The relatively high photon energy of 20 keV was chosen to penetrate the 500 $\mu$m wide guard ring, which is an insensitive region of the sensor. The sensor depth of 320 $\mu$m was scanned in 10 $\mu$m steps. At the backplane ($z = 0$) the charge cloud drifts through the entire sensor material, whereas closer to the electrode ($z = 300$ $\mu$m) the drift time is shorter. A 3-axis rotation stage enabled precise parallel alignment of the detector surface to the beam. Two different sensor bias voltages of 90 V and 120 V were used, to investigate the charge drift at different electrical field strengths [53]. At each step $500 \times 10^3$ frames with an exposure time of 12 $\mu$s were acquired. The short exposure time gives a high detector dead time of $\sim 99 \%$. The acquisition length for one scan step was 500 s at 1 kHz frame rate. About $1.22 \times 10^6$ counts are detected per scan step with
Figure 6.3: (a) noise map of the first super-column of MÖNCH. (b) pedestal plot for three random pixels (circled in (a)) with the Gaussian fitting function (dashed). The black line represents the fit for all pixels. (c) projection of noise map onto the y-axis. The signal droop causes a small reduction of the noise, if the pixel signal is read-out later.
a step-to-step fluctuation of $\pm 89 \times 10^3$ for the scan at 90 V bias voltage. At 120 V $1.12 \times 10^6$ counts were detected, with a fluctuation of $\pm 89 \times 10^3$ [53].

Figure 6.5: Setup of the sensor depth scan performed at SYRMEP: A collimated 20 keV beam (5 $\mu m$) is aligned horizontally to the sensor surface and scanned vertically through the sensor volume. Schematic representation, not to scale [53].

Figure 6.6 shows the spectrum of the center pixel of the cluster at different absorption depths and the average spectrum at all absorption depths. The results for the two measurements at 90 V and at 120 V bias are plotted in figure 6.6a and figure 6.6b, respectively. The center pixel receives, by definition of the cluster, the most charge of all pixels in a cluster. The spectra are normalized, so that the total counts accumulate to 1. The fraction of the collected charge is low for both measurements, if the photon is absorbed close to the backplane (low $z$ value). If the absorption of the photon is closer to the read-out pad (i.e. high $z$ value), the charge of more absorption events are collected in the center pixel entirely. This is caused by the large area of the charge cloud after the long drift time of 150 $\mu m$ and more, and is visible in these figures, by the peak close to 2000 ADUs, which is only present in spectra with $z > 160 \mu m$. The cumulative spectra at all absorption depths (dashed black lines) match well with the theoretical charge sharing model.
shown in section 3.3.

Figure 6.7 shows a comparison of the spectra acquired with 90 V (solid lines) and 120 V (dashed lines) bias voltage for four different absorption depths. Shown are the spectra for the center pixel (equivalent to figure 6.6) in blue and the sum of all pixels of the $2 \times 2$ (in red), $3 \times 3$ (in green) and $5 \times 5$ (in yellow) clusters.

If the drift time is long (low $z$) the difference between the two bias voltage settings is bigger, then at short drift times (compare figure 6.7a and figure 6.7d). This is caused by more diffusion at lower bias, if the drift time is longer. If the drift time is short, the difference of the diffusion has lower impact.

The center pixel spectra at $z = 0 \mu m$, $z = 100 \mu m$ and $z = 200 \mu m$ show that at higher bias voltage more charge is collected by the center pixel, while at a short drift distance ($z = 300 \mu m$) there is no difference visible in the center pixel spectra.

At all absorption depths, the noise of the signal increases, if more pixel values are summed (i.e. bigger cluster size). Figure 6.7 indicates this with broader peaks for bigger clusters.

In figure 6.8, the total collected charge of $2 \times 2$, $3 \times 3$ and $5 \times 5$ pixel clusters (at scan position $z$) $Q(z)$ is compared to the total sum of $5 \times 5$ clusters at $z = 300 \mu m$ (denoted $Q_0$) for two bias voltages [53]. It is assumed that $Q_0$ contains all the charge produced by the photon hit [53]v. The plot shows that close to the charge collection implant ($z = 0$) all cluster sizes collect the full charge. At larger distances the small cluster sizes loose more charge than the large ones and the collected charge at 120 V is for any cluster size higher than for the same cluster size at 90 V. These effects can both be understood as an increase in the size of the charge cloud caused by the longer drift times of the signal charge at larger distances or smaller bias voltages. For larger drift times the charge cloud will also be larger, due to diffusion and in smaller clusters more charge will be lost. Currently, it is not clear what causes the signal loss at small $z$ for the $5 \times 5$ cluster. Close to the electrode the collected charge difference gets smaller between different cluster sizes and different bias voltages. The charge collection characteristics for $2 \times 2$ clusters has a non-linear dependency of the absorption depth $z$. At the backplane 13 % and 9 % of the charge...
Figure 6.7: Comparison of the center pixel, 2 × 2, 3 × 3 and 5 × 5 pixel cluster spectra for two different sensor bias voltages, at an absorption depth of \( z = 0 \) µm (a), \( z = 100 \) µm (b), \( z = 200 \) µm (c), and \( z = 300 \) µm (d).

is not collected by the small 2 × 2 cluster for a 90 V and 120 V sensor bias, respectively [53]. This may show that bigger clusters are beneficial for position reconstruction for lower X-ray energies or thicker sensors. Though, the noise introduced by the analog circuitry increases as well with bigger cluster sizes in these scenarios.

In figure 6.9, \( \eta \)-distributions (see section 4.2 for a detailed explanation) for different interaction depths are plotted. A small fraction of the events are outside the expected range of \( \eta = (0,1) \). This occurs if, the charge induced by a photon absorption is detected by only one pixel and all the adjacent pixels sample negative noise in this particular frame. It is also clearly visible that for higher \( z \) values, the peaks at the border are more prominent. Since the total amount of counts \( N \) is similar for all absorption depths, less counts are present in the center of the \( \eta \)-distribution [53]. The shoulder of the peaks (most prominent for the averaged distribution in figure 6.9) is a geometric effect, and can be investigated by using more complex charge collecting models (see section 6.1 and [77]). For \( z = 0 \) hits with \( \eta \) close to 0 or 1 are rare, because the charge cloud diffuses more
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Figure 6.8: Comparison of the average collected charge in $2 \times 2$, $3 \times 3$ and $5 \times 5$ clusters at different interaction depths for two different sensor bias voltages [53].

and is never detected by only one pixel [53].

For hybrid detectors, the $\eta$-parameter is dependent on the absorption position in a non-linear way. To quantify the non-linearity of the $\eta$-parameter, the peak-valley ratio ($PVR$) of the $\eta$-distribution was investigated:

$$PVR = \frac{\max_{\eta} \left( \frac{dN}{d\eta} \right)}{\min_{\eta} \left( \frac{dN}{d\eta} \right)}.$$

In general a $PVR$ close to 1 (indicating a flat $\eta$-distribution) shows that the investigated clusters contain a more linear position information, and therefore the position reconstruction is simpler [53].

Another method to quantify the size of the area where charge sharing occurs, and therefore position information is available is explained in [98].

Figure 6.10 shows the absorption depth ($z$) dependent $PVR$s (denoted as $PVR(z)$). The $PVR(z)$ for 120 V bias voltage is on average 30% higher than for 90 V bias voltage. This is mostly due to the faster charge collection time at higher electric field strengths. The $PVR$ at $z = 300 \mu m$ for 90 V bias voltage is 47 times (35 times for 120 V) higher than at $z = 0$. If the photon interaction is further away from the electrode the $PVR$ is lower and therefore the events contain more usable position information. One can further conclude that thicker sensors would have more volume with low $PVR$ and the position resolution is less dependent on the interaction depth [53]. The average absorption depth is smaller for lower energies and the $PVR$ is also lower.
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Figure 6.9: $\eta$-distribution at different interaction depths at 90 V bias voltage. The shape of the distribution changes, although the total amount of detected photons remains constant [53].

6.5 Position resolution measurements

To evaluate the position resolution of the MÖNCH detector together with the position interpolation algorithms developed during this thesis (see chapter 4), an edge scan was performed at the Synchrotron Radiation for Medical Physics (SYRMEP) beamline, Elettra Sincrotrone, Trieste, Italy [97]. A steel edge with polished surfaces that was specifically manufactured for this measurement, was placed in the beam in front of the detector (see figure 6.11). The edge was inclined to the pixel matrix of the detector, such that it covered two pixels of 25 $\mu$m pitch over the entire field of view of 4 mm (see figure 6.12a). There were $2.5 \times 10^6$ frames with an exposure time of 12 $\mu$s (total exposure time: 30 s) recorded for the beam energies 10 keV, 12 keV and 16 keV and at two different bias voltages for the detector (90 V and 120 V). I.e. 6 measurements in total were performed. The beam was attenuated with 2.5 mm aluminum, resulting in an average beam intensity over all 6 measurements of $\sim 10 \times 10^6$ photons $mm^{-2} s^{-1}$ (not corrected for sensor efficiency).

Figure 6.12a shows the image of the acquisition with the 12 keV beam and a bias voltage of 90 V. The measurement for the other energies and bias voltage look comparable and are therefore not depicted. The position resolution is dependent on the in-pixel position, i.e. the resolution is higher at pixel borders (dashed blue lines indicate the horizontal pixel borders) and lower at pixel centers. Additionally, the interpolated image is shifted by a fraction of the pixel pitch to the right (towards higher x-values), since there is cross talk in the analog read-out electronics of the detector. The pixels are read-out in a serial fashion in x direction. The cross talk is originating from a too slow off-chip driver, which leads to a signal convolution of the current pixel with the previously read pixel signal. To account for the different in-pixel spatial resolution responses of the
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Figure 6.10: Change in $\eta$-distribution uniformity represented by the peak-value-ratio $PVR(z)$ at different interaction depths. Uniform $\eta$-distributions have a $PVR(z)$ equal to 1. (a) linear, (b) logarithmic representation [53].

detector, several regions are defined and the position resolution analysis was performed on each of this regions individually. The three regions are depicted in figure 6.12a with colored rectangles. The region $R_L$ is chosen, such that the edge of the sample is in a position, relative to the vertical pixel position, where the expected resolution is low. $R_H$ is placed, in a in-pixel position, where a high resolution is expected, and $R_T$ is chosen, such that it covers one pixel in horizontal direction completely. The positions of the regions are chosen by hand for each of the 6 measurements separately, since there was a slight shift of the edge in the x-direction between the measurements.

To evaluate the position resolution, each pixel value of a region is projected to the x-axis, where at the red line in figure 6.12a indicates 0. The projected points are then fitted with an error function and the $\sigma$-value of the fitted function represents the position resolution in that region. This is repeated for all energies, bias voltages and regions. The results are depicted in figure 6.12b.

In the best case, the resolution was 3 $\mu m$ in the $R_H$ region at 10 keV. In regions, where charge sharing between pixel is limited, the resolution goes up to 6.4 $\mu m$. At high energies of 16 keV, lower bias voltage yields better results, whereas at 10 keV higher bias voltages are beneficial. For the photon energy there is no trend determinable in terms of position resolution. Note that, the spatial resolution of a pixelated detector with a pixel pitch of $p = 25 \mu m$ is limited to 7.22 $\mu m$ (see section 2.3.2). However, by analyzing the charge shared between pixels for individual photons, it is possible to improve the spatial resolution below this limit, as it is demonstrated with this experiment.

6.5.1 Angular alignment

The angular alignment of the detector surface perpendicular to the beam direction has an influence on the spatial resolution. To investigate the impact a short calculation is performed. Figure 6.14a
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Figure 6.11: Edge experiment setup. Picture taken along the beam path. In front the steel edge is visible. In the background one can see the PCB with the MÖNCH prototype chip.

Figure 6.12: (a) is an overview of the knife edge measurement. Depicted is the result for a 12 keV beam and a bias voltage of 90 V. The dashed blue lines indicate the pixel border. The red line indicates 0 for the projected pixel values. Three regions are investigated: $R_L$ is the region with low position resolution; $R_H$ is the region with highest position resolution; and $R_T$ is an average over the full pixel width. Note that the edge is rotated counter-clockwise by 90° to the experimental setup depicted in figure 6.11. (b) Resolution measurement for the different regions, bias voltages and energies.
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shows the absorption probability density function (PDF) for three different energies with a sensor thickness of \( d = 320 \mu m \). At low energies the sensor thickness has low impact, and therefore the PDF for \( d = 450 \mu m \) is only plotted for 30 keV. It also indicates the mean absorption depth (marker) and the standard deviation of the absorption depth (error bar). The sensor material considered in this calculation is silicon.

![Diagram showing the absorption probability density function (PDF) for three different energies with a sensor thickness of \( d = 320 \mu m \).](image)

Figure 6.13: Variable declaration of the angular alignment simulation.

Figure 6.13 shows the variable declaration for the performed simulation. If the beam travels parallel to \( z \) through the sensor with thickness \( d \), the absorption probability can be modeled with a truncated exponential (TEXP) PDF:

\[
\frac{dP(z)}{dz} = \frac{\mu/\rho e^{-\mu/\rho z}}{1 - e^{-\mu/\rho d}}, \tag{6.2}
\]

where \( \mu \) is the mass absorption coefficient of the sensor material and \( \rho \) the density of the material. If the beam is inclined to the sensor surface normal by the angle \( \alpha \), the resulting spatial error can be estimated by projecting the PDF in equation 6.2 to the sensor surface (x-axis) and by calculating the standard deviation of the resulting projected PDF. If \( E(P) \) is the expected value of the probability variable \( P \), the standard deviation of a TEXP is given by [99]:

\[
\sigma = \sqrt{E(P^2) - (E(P))^2}, \tag{6.3}
\]

where

\[
E(P) = \lambda \left[ \frac{1 - (k + 1)e^{-k}}{1 - e^{-k}} \right],
\]

\[
E(P^2) = 2\lambda^2 \left[ \frac{1 - \frac{1}{2}(k^2 + 2k + 2)e^{-k}}{1 - e^{-k}} \right], \tag{6.4}
\]

with

\[
\lambda = \frac{\rho}{\mu} \quad \text{and} \quad k = \frac{d\mu}{\rho} = \frac{d}{\lambda}. \tag{6.5}
\]
To get the variance of the PDF projected to the sensor surface, $\lambda$ is corrected by:

$$\lambda' = \frac{\rho}{\mu} \sin \alpha.$$  \hspace{1cm} (6.6)

The correction factor of $k$ cancels out. If the beam direction is inclined to the sensor surface, the path length of the beam in the sensor bulk prolongates by $d' = d / \cos \alpha$, where $d'$ is the inclined beam path length. Since $\alpha$ is close to 0, this was not considered in the following calculation, and $d' \approx d$ was assumed.

Figure 6.14b shows the standard deviation, and therefore the error on the position, introduced by the angle of the beam. The values are plotted up to 10 mrad. At low energies, the sensor thickness has low impact on the average absorption depth. At higher energies, the average absorption depth moves to the center of the sensor volume and the standard deviation gets bigger. At low energies, the impact is not significant and similar for both sensor thicknesses. Although at higher energies, the thicker sensor is beneficial in terms of absorption efficiency, it has higher sensitivity to alignment errors. Note that the thicker sensor with $d = 450 \mu m$ is more sensitive to alignment errors at 10 keV, than the thinner sensor (with $d = 320 \mu m$) is at 30 keV.

Figure 6.14: (a) shows the absorption probability density function for two sensor depths at different energies. The marker indicates the average absorption depth and the error bar the variance. The lines for 450 $\mu m$ at 8 keV and 10 keV are omitted, since they are similar to the same energy at $d = 320 \mu m$. (b) shows the error introduced by the angle of the incident beam to the surface of the detector.
Chapter 7

Absorption imaging with GOTTHARD and MÖNCH

During the test phase of GOTTHARD and MÖNCH various absorption imaging experiments were performed. The purpose of these experiments was to have real data for testing the various high-resolution imaging algorithms and to gain experience about the usability of the detectors in different setups. In this chapter we show some of the imaging results. Additionally, experience with polychromatic X-rays from an X-ray tube was gained. In the last part we show some initial results from an energy dispersive experiment.

7.1 General setup

The experiments requiring a synchrotron source were performed at the Tomcat beamline at the Swiss Light Source. This beamline was chosen because it is an imaging beamline with a low beam divergence and a monochromatic beam. Because operating the detectors in the single-photon regime requires low photon intensities, the high brilliance of the source was an unwanted property. Therefore, the beamline was operated with the Si[111] monochromator instead of the also available multi-layer monochromator. Si[111] has a bandwidth of $\Delta E / E = 10^{-4}$, giving a very narrow-bandwidth beam and also low flux. To further reduce the flux, 2 mm of aluminum was placed after the source. If not other mentioned the beam energy is 16.7 keV.

The GOTTHARD strips have a length of 8 mm, therefore for two-dimensional imaging an aperture with a 2 $\mu$m opening in vertical direction was placed 1 mm in front of the detector. With this method it was possible to scan the sample in 2 $\mu$m steps resulting in a high resolution in vertical direction. A multi-pitch sensor with strips from 10 $\mu$m up to 100 $\mu$m was available, however only the region with 25 $\mu$m was used during these experiments.

The currently used MÖNCH detector (MÖNCH 0.2) is a test chip with 5 kind of pixel architectures on one chip. Each super column (SC1 to SC4) has a different type of pixel architecture. SC1 has pixels with an architecture optimized for single-photon imaging. Therefore for the presented experiments this super column was used. The resulting images have a size of $1 \times 4 \text{ mm}^2$. Future imaging experiments will be performed with a new version of MÖNCH having only this type of pixel architecture and a field-of-view of $10 \times 10 \text{ mm}^2$. 
CHAPTER 7. ABSORPTION IMAGING WITH GOTTHARD AND MÖNCH

7.2 Medical sample imaging

For this experiment kidney stones of roughly $1 \times 1 \text{ mm}^2$ were used. They have fine pitch features down-to the micrometer level and are therefore ideal for testing the high-resolution algorithms. The experiment was performed with MÖNCH and GOTTHARD at different times, hence two different samples were used. For both detectors the standard setup at the Tomcat beamline was used.

For the acquisition with the strip detector the sample was stepped through the beam in 500 steps of 2 $\mu$m. Per step $500 \times 10^3$ frames with an exposure time of 1 $\mu$s were acquired. Additionally, for a flat-field correction and also to calibrate the interpolation algorithm, $500 \times 10^3$ frames of flat-field were acquired.

Figure 7.1 shows the acquired image with GOTTHARD. For both version (i.e. figure 7.1a and figure 7.1b) the same data-set was used. After applying the interpolation algorithm much more details are visible. The image before interpolation (see figure 7.1a) has a pixel size of $25 \times 2 \mu$m. This is given by the physical pitch of the detector in horizontal direction, and by the $2 \mu$m scanning steps in vertical direction.

The interpolated version in figure 7.1b has a pixel size of $2 \times 2 \mu$m. The vertical lines visible in-between strips originate from the high amount of charge sharing between neighboring strips. In these regions, the position resolution is higher and more detailed features are visible. With a simple image-processing filter (for example Gaussian blurring) the resolution in this area could be reduced and the image resolution would be lower but uniform in all image regions.

With MÖNCH a total of $65 \times 10^6$ photons in $10^6$ sub-frames were detected. Additionally, the same amount of flat-field data was recorded. The flat-field contains $100 \times 10^6$ photons.

Figure 7.2 shows a kidney stone sample, acquired with MÖNCH. The field-of-view of the image is $1 \times 4 \text{ mm}^2$. Figure 7.2a shows the data-set represented only by the physical pixel information, therefore the pixel size is $25 \times 25 \mu$m. Figure 7.2b shows the same data-set after resolution interpolation with an virtual pixel size of $1 \times 1 \mu$m. We assume, that the dark spots visible in the lower right corner originate from pixels with constant lower signal response, since they are not visible in the low-resolution version of the same data-set. The event count per virtual pixel in the position interpolated version is reduced by a factor of $25 \times 25 = 625$, hence the pixel-to-pixel noise is higher and well visible in the background. Increasing the acquisition time and therefore the statistics would reduce this Poisson noise.

7.3 Tomography with biological sample

We conducted this experiment with GOTTHARD to demonstrate the feasibility of tomographic absorption imaging with a charge integrating strip detector operated in the single photon regime. Only one tomographic slice was acquired. The sample is a toothpick with a diameter of $\sim 750 \mu$m. To simplify the positioning of the sample in the beam, a strongly absorbing steel needle was mounted next to the toothpick.

The experiment was performed at the Tomcat beamline at 12 $keV$. Again the collimating aperture in front of GOTTHARD was used. Instead of scanning the sample vertically, it was rotated by 1200 small steps of 0.15°, resulting in a $180^\circ$ total angular coverage. $300 \times 10^3$ frames were recorded per projection step. With an exposure time of $1 \mu$s, the total exposure per projection was 3 s. For the tomographic reconstruction, a publicly available software library was used [100].

The left side of figure 7.3 shows a low and a high-resolution sinogram, where all projections
7.3. TOMOGRAPHY WITH BIOLOGICAL SAMPLE

Figure 7.1: A kidney stone acquired with GOTTHARD from a 15 keV beam. In (a) the resolution in horizontal direction is given by the strip pitch of 25 $\mu m$. In the vertical direction the sample was stepped in 2 $\mu m$ steps, giving the vertical resolution for (a) and (b). In (b) the interpolated position in horizontal direction is used and the image is binned in $2 \times 2 \mu m^2$.

Figure 7.2: A kidney stone acquired with MÖNCH from a 16.4 keV beam. (a) shows the image with the resolution of the physical pixel size of the detector. The pixel size is $25 \times 25 \mu m^2$. (b) shows the image after the position integration. The pixel size is 1 $\mu m^2$. 
Figure 7.3: Sinogram and tomographic reconstruction of one slice of a wood sample with a diameter of 750 µm. (a) and (b) show the sinogram with 1200 projections (low and high resolution version). (c) is the reconstructed slice from the 1200 projections.

of one slice are stacked vertically. In figure 7.3a channel 32 is a copy of channel 33. This results from a bug in the used firmware version of the GOTTHARD detector and was corrected after the experiment. In figure 7.3b this bug translates in two high intense vertical lines and additional distortions around these channels.

Figure 7.3c is the reconstructed slice from the sinogram visible in figure 7.3b. The image center is also the rotation center. Since the sample was not completely in the field of view for all projections, the reconstruction has some artifacts. The strong absorbing steel rod also introduces artifacts in its proximity. Some structure of the wood is visible. Particularly some mostly pairwise arranged hollow tubes, presumably for water and nutrition transport. To reduce artifacts in the reconstruction the previously mentioned high intensity regions around channels 32 and 33 were eliminated by applying an image filter in these regions.
7.4 MÖNCH and Nanoscopium

The Nanoscope setup at the Tomcat beamline of the Swiss Light Source is a hard X-ray microscope with a resolution around 100 nm. This high resolving power is achieved by focusing the beam with Fresnel zone plates (FZPs). The efficiency of FZPs at the experimental energy of 16 keV is low and therefore the beam intensity at the detector plane is also low. Integration times up to minutes are required with indirect detection microscopes. Mainly because of their high quantum efficiency and good position response charge integrating hybrid detectors are well suited for such low intensity tasks. Therefore, we tested MÖNCH as a detector for the nanoscope and performed a comparison with a CCD detector.

The field of view is limited by the optical arrangement to $2.75 \times 2.75 \text{ mm}^2$ at the detector plane, resulting in a field of view of $33 \times 33 \text{ µm}$ at the sample. The sample was an absorbing Siemens star with 0.5 µm gold plating on a silicon wafer. The smallest features of the Siemens star have a size of lower than 100 nm.

Since the magnification of the microscope is a factor of 83, the MÖNCH detector with a pixel size of 25 µm has a 300 nm pixel size at the sample plane. The exposure time was set to 12 µs per sub-frame. With $10^6$ sub-frames, the length of the aggregated exposure was 120 s.

For comparison of the resulting image quality we replaced the MÖNCH detector with a high sensitivity Photonics Science VHR water cooled CCD detector. This detector has a 14-bit dynamic range and is coupled via a fiber optics taper (with 3-fold magnification) to the scintillator screen. The geometrical pixel size at the scintillator plane is 4 µm [101]. With the magnification this results in a pixel size of 48 nm at the sample plane.

Figure 7.4 shows the resulting images of a small fraction of the Siemens star acquired with both detectors with an equal exposure time of 120 s. Although, the pixel size at the sample plane is larger with MÖNCH than with the CCD detector, the image produced by MÖNCH is less blurred (see figure 7.4a). We assume that the blurring in figure 7.4b originates from the high sensitive scintillator, which is relatively thick and has therefore a low point-spread function (PSF), while the PSF of MÖNCH is most probably not the limiting factor of the experimental setup. Because of the limited field-of-view of the MÖNCH detector in combination with the microscope, only $2.75 \text{ mm} \times 1 \text{ mm}$ at the detector plane could be used for imaging. Therefore, vertical stitching of 5 images was required. Whereas, stitching of two images was enough with the CCD camera, since it covered the full $2.75 \text{ mm} \times 2.75 \text{ mm}$ projected by the optics. The microscope optics introduced image distortions which are more prominent with more stitching. Therefore, the image acquired with MÖNCH looks more distorted than the one acquired with the other device. The four black spots in the top left of each stitched frame in figure 7.4a are the result of two dead pixels in the used MÖNCH detector. After interpolation, they expand to distortions with a size of the physical pixel size.

To evaluate the spatial resolution of the microscope with the two detector systems, an edge was fitted with the error function (see figure 7.5). Figure 7.5a and figure 7.5b show the area of the images in figure 7.4, where the resolution measurement was performed. The red and yellow line are placed by hand and indicate the edges between the absorbing and the transmitting part of sample. The distance between the lines is 1 µm. The intensities of the pixels in the blue rectangles are projected on the x-axis, while the red line indicates 0 and the yellow line indicates 1 µm. In figure 7.5c and figure 7.5d the projected intensities are depicted. The spatial resolution was evaluated by fitting an error function to these data points. The $\sigma$ of the function fit is considered as the spatial resolution. The measured resolution of the microscope and the Photonics Science CCD detector is $\sigma_C = 83.5 \text{ nm}$ at the sample plane. In comparison, the resolution of the instrument...
Figure 7.4: Sample acquired with the nanoscope at Tomcat with two different detectors. (a) shows the image produced with MÖNCH and (b) shows the image acquired with the Photonic science CCD detector.
with MÖNCH is $\sigma_M = 65.3 \text{ nm}$.

With this experiment we could demonstrate, that the MÖNCH detector gives a higher spatial resolution than the previously used water cooled CCD detector, with the same acquisition time.

### 7.5 Energy sensitive imaging with MÖNCH and an x-ray tube source

To demonstrate the possibility of energy sensitive imaging with hybrid detectors, we used an X-ray tube as a polychromatic source, during this experiment. The tube current was tuned such that we could operate MÖNCH in the single photon regime. The high voltage was set at $35 \text{ kV}$ and therefore, the tube produced photons up to $\sim 35 \text{ keV}$.

To collimate the beam and reduce the flux we placed a small aperture of $1 \text{ mm}$ diameter after the source. The sample was at a distance of $\sim 1 \text{ m}$ and the detector $1 \text{ cm}$ behind the sample. With this setup, the beam divergence at the detector could be reduced to $1 \text{ mrad}$ and is below the physical pixel size of the detector.

For this experiment $10^7$ sub-frames at an exposure time of $12 \mu\text{s}$ each were recorded. Resulting in a total amount of recorded photons of $116 \times 10^6$. Note that the polychromatic photons were recorded at the same time without altering the experiment nor the settings of the detector. The energy binning of the resulting images can be done offline from the recorded data.

The sample consisted of various metal chips (steel, aluminum and copper) of different thicknesses and different materials. The metal chips are placed on a Kapton foil and have feature sizes ranging from $25 \text{ \mu m}$ up to $1 \text{ mm}$. Figure 7.6a shows an x-ray image, where photon hits in all energy ranges are plotted for each pixel. There are four regions with different materials marked in the image. Region $R_1$ is the unchanged radiation of the x-ray tube. Region $R_2$ is an aluminum alloy, where we assume that it contains Nickel. Region $R_3$ is the copper wool, and region $R_4$ is a steel chip.

Figure 7.7a shows the four different spectra of the regions indicated in figure 7.6a. The spectra are normalized to counts per pixel and $\text{keV}$, to take the different regions sizes into account. To amplify the difference induced by the materials, we divided the spectra of region $R_2$ to $R_3$ by region $R_1$ (see figure 7.7b). There are three distinct peaks visible in the divided spectra. The peaks are due to fluorescence of the different materials. By fitting these peaks and the additional one originating from the x-ray tube target at $9.67 \text{ keV}$, it was possible to calibrate the energy response of the detector. Figure 7.8 shows the linear calibration fit for the four known material emission lines. Note that the error bars of the peak fits in figure 7.7a and figure 7.7b are quite big and the energy calibration is not very precise. However, for this initial experiment we decided, that it is sufficient. For comparison, a calibration of the same detector module presented in [19] is plotted as dashed black line. The spectrum is not corrected by the silicon sensor efficiency.

To generate the energy dependent color image in figure 7.6b the HSL-color-model [102] was used. This color model uses the three values: Hue, Saturation and Lightness to represent a color. The conversion from HSL-values to the red, green and blue values of the RGB-color-model is straightforward and explained in [102].

In figure 7.7b three energy bins named $B_1$, $B_2$ and $B_3$ are indicated. The center of the bins $B^C_n$ are the peak centers of the three materials present in the regions $R_2$, $R_3$ and $R_4$. The border of the energy bins are in the middle of two neighboring bin centers. Each pixel at position $(x,y)$ has four intensity count values. $I_T^{x,y}$ are the total counts over the entire energy range. $I_1^{x,y}$, $I_2^{x,y}$ and $I_3^{x,y}$ are the counts in the energy bin $B_1$, $B_2$ and $B_3$, respectively. The saturation value of the
Figure 7.5: Spatial resolution measurement of the Nanoscopium. (a) and (b) show the region, where the resolution measurement was performed. The distance between the red and yellow line is 1 \( \mu m \) and was used to project the line points. The blue region indicate the pixels used for the measurement. (c) and (d) show the projected point of the blue region. The edge along the red line is fitted with an error function.
7.5. ENERGY SENSITIVE IMAGING WITH MÖNCH AND AN X-RAY TUBE SOURCE

HSL-color-model is kept constant at $S_{x,y} = 1$. The lightness is calculated by the total intensity:

$$L_{x,y}(I_{x,y}^T) = \frac{I_{x,y}^T}{\text{max}_{x', y'}(I_{x', y'}^T)},$$

(7.1)

i.e. the total intensity is normalized between 0 and 1. Finally, the hue value is the normalized weighted average of the three bin centers. The weighted average before normalization is evaluated by:

$$\hat{E}_{x,y}(I_{x,y}^N) = \frac{\sum_{n=N} I_{x,y}^n B_C^C}{\sum_{n=N} I_{x,y}^n}$$

(7.2)

and

$$\hat{E}_{x,y} = \frac{I_{x,y}^1 B_C^C + I_{x,y}^2 B_C^C + I_{x,y}^3 B_C^C}{I_{1}^x + I_{2}^x + I_{3}^x}.$$  

(7.3)

And $\hat{E}$ is normalized by the minimum ($\hat{E}_{\text{min}}$) and maximum value ($\hat{E}_{\text{max}}$) of all pixels:

$$H_{x,y}(\hat{E}_{x,y}) = \left( \hat{E}_{x,y} - \hat{E}_{\text{min}} \right) \left( \hat{E}_{\text{max}} - \hat{E}_{\text{min}} \right).$$

(7.4)

The energy range covered by the hue value is indicated in figure 7.7b in the bottom.

Region $R_4$ and the rest of the iron pieces have a low weighted average energy level around 6.5 keV. Therefore, they appear reddish and greenish in figure 7.6b. The hue-value is not stable because the photon counts and therefore the statistics are low due to absorption. Region $R_2$ and $R_3$ have a higher x-ray emission line and appear therefore blue and violet. While the two iron pieces are almost fully absorbing over the entire energy range, the aluminum coil and the copper wool are more transparent at higher energies. The border of the iron pieces appear to be rather thin and therefore high energies still penetrate the object (note the slight shift towards blue in figure 7.6b). There are several dead pixels, with a random energy response, visible in the acquisition.
Figure 7.6: Image of a measurement of two iron pieces ($R_4$), an aluminum coil ($R_2$) and copper wool ($R_3$). (a) image without energy discrimination. The energy spectra of the regions indicated ($R_1$-$R_4$) are shown in figure 7.7. (b) has the energy response encoded in the color. The coloring was done with the HSL-color model (see text).
7.5. ENERGY SENSITIVE IMAGING WITH MÖNCH AND AN X-RAY TUBE SOURCE

Figure 7.7: (a) acquired spectra for the four different regions indicated in figure 7.6a. (b) spectra of three regions divided by the flat region $R_1$. $B_1 - B_3$ indicate the three energy bins, that are used to generate the hue value of figure 7.6b. The dashed lines are the Gaussian fits to evaluate the centers of the energy bins $B_1 - B_3$ and to perform the energy calibration of the detector. The hue to photon energy mapping is indicated in the bottom of the plot.

Figure 7.8: Energy calibration of the detector. The analog digital units can be calibrated to photon energies, by fitting the tube spectrum of region $R_1$ and the three different materials in regions $R_2$ to $R_3$ (blue line). The error bars represent the sigma of the fits shown in figure 7.7a and figure 7.7b. We assume that the aluminum in region $R_2$ is an alloy containing nickel. The black line represents the energy calibration done by [19].
Chapter 8

$G_2$-less grating interferometer experiments

In this section, we describe two experiments that explore the possibilities of performing phase sensitive imaging with silicon hybrid detectors. In particular, a grating interferometer without an analyzer grating $G_2$ was setup at the TOMCAT beamline. The working principle of the $G_2$-less grating interferometer is explained in section 5.5. The TOMCAT beamline and parts of the used setup are described in section 7.1. In section 8.1 a initial experiment with the GOTTHARD strip detector (see section 3.5) is described, and in section 8.2 a similar experiment with a pixel detector (see section 3.6) is shown. The experiment was initially performed with a strip detector with a vertical stepping to acquire a two-dimensional image, since the fine pitch pixelated detector was not available in the beginning. Parts of the following sections are reprints of the two publication. Particularly, the experiment with the strip detector is described in [96], and the final experiment with the pixelated detector is shown in [19].

8.1 $G_2$-less grating interferometry with a strip detector

The Si(111) monochromator of the TOMCAT beamline at the Swiss Light Source was set to 16.7keV. The beam was attenuated by a 50% filter and a 350m aluminum sheet to enter the single photon regime. A silicon $\pi/2$ phase grating (produced at the Laboratory for Micro and Nanotechnology (LMN) of the Paul Scherrer Institute, Villigen, Switzerland) with a pitch of 4.7 $\mu$m was placed behind the sample of investigation. The GOTTHARD detector was mounted at the first Talbot distance ($\sim 15$ cm) behind the phase grating. The equally segmented 320 m thick silicon sensor of GOTTHARD gives a detection efficiency of 59% at the X-ray energy of 16.7 keV. GOTTHARD can readout a selected region of 256 strips at 140kHz frame rate. In the experiment, a region of 31 strips with a pitch of 25 $\mu$m was used. This corresponds to a field-of-view of 775 $\mu$m. Each channel was subdivided into 64 virtual channels, resulting in a total of 1984 virtual channels. The investigated sample was a polyethylene (PE) sphere (Cospheric LLC, Santa Barbara, CA 93160, USA) with a diameter of 625 $\mu$m mounted on the tip of a steel needle. A two-dimensional image was acquired by scanning the object vertically through the beam in 30 steps of $q = 25$ $\mu$m. Fifty millions frames of an exposure time of 1 $\mu$s were acquired per measurement. This resulted in a total scan time of about 3 h per image. This very long exposure time is mainly given by the long dead time determined by the low flux required by the detector to perform interpolation on single photons [96].
With the virtual channels of each detector channel, one differential phase value (and one absorption value) was evaluated. For this, the sample intensity curve (i.e., \( I^{c}_{s}(x) \)) and the grating intensity curve (i.e., \( I^{c}_{g}(x) \)) were obtained for each channel pair \( c \), after the position interpolation. The absorption and differential phase values were then calculated by using the algorithms described in section 5.6.3 for each channel couple \( c \) individually. Figure 8.1 shows the resulting contrasts. Figure 8.1a shows the absorption contrast and figure 8.1b the differential phase contrast.

To make a quantitative comparison the differential phase contrast for a PE sphere with the same diameter was calculated (see figure 8.1c). The distance \( \Delta z \) traveled in the sample at position \((x, y)\) is given by:

\[
\Delta z(x, y) = 2\sqrt{r - x^2 - y^2}, \tag{8.1}
\]

where \( r \) is the radius and \( x \) and \( y \) is the distance to the center in \( x \) and \( y \) direction, respectively. Reconsidering equation 5.16 in section 5.1, the phase shift given by the path length \( \Delta z \) can be evaluated for all positions in the \((x, y)\) plane after the sample:

\[
\Delta \Phi(x, y) = \left( \frac{2\pi\delta}{\lambda} \right) 2\sqrt{r - x^2 - y^2}, \tag{8.2}
\]

where \( \delta \) is the refractive index of PE. Thus, the differential phase shift in \( x \) direction is given by:

\[
\frac{d\Phi(x, y)}{dx} = \frac{4\pi\delta}{\lambda} \frac{x}{\sqrt{r - x^2 - y^2}}. \tag{8.3}
\]

For a phase shift grating with pitch \( g_1 \) at the distance \( z_T \) the fringe shift introduced by the sample is:

\[
\Delta \varphi = \frac{z_T\lambda}{g_1} \frac{d\Phi(x, y)}{dx} = 4\pi \frac{z_T\delta}{g_1} \frac{x}{\sqrt{r - x^2 - y^2}}, \tag{8.4}
\]

where \( z_T = 15.7 \text{ cm}, g_1 = 4.7 \mu m \) and \( \delta = 8.1631 \times 10^{-7} \) for PE at 16.7 keV. Figure 8.1d shows a comparison of the line profile of the pixel line indicated in figure 8.1b and figure 8.1c.

### 8.2 \( G_2 \)-less grating interferometry with a pixel detector

Figure 8.2 shows the simplified grating interferometer used at the TOMCAT beamline. The sample was illuminated with an 16.7 keV beam. The phase grating \( G_1 \) can be placed before or after the sample. And the MÖNCH detector was placed at a distance \( z_T = 15 \text{ cm} \) from \( G_1 \). The beam was bandwidth limited with a Si(111) monochromator and additional filters were introduced to operate MÖNCH in the single-photon regime. A 4.7 \( \mu m \) pitch \( G_1 \) silicon phase grating with a duty cycle of 50% and a depth of 33 \( \mu m \), introducing a phase shift of \( \pi/2 \) was used for the experiment. The grating was produced at the Laboratory of Micro and Nano technology of the PSI [19].

Three measurements are performed for calibrating the experiment and acquiring sample data. The blank measurement is used to populate the correction map for the interpolation algorithm. The grating measurement for acquiring the fringe pattern without distortions from the sample. And finally, the sample measurement, where the fringes with the distortions from the sample are recorded. Due to the limited frame rate of the current detector prototype, each of the three images required for the experiment took about three hours, using a sub-frame exposure time of 12\( \mu s \) and frame rate of 1 kHz, i.e. the sensor is insensitive 99% of the time due to the speed of the current
Figure 8.1: Polyethylene sphere of 625 µm diameter acquired with the proposed method. (a) Absorption signal $A^c$, (b) differential phase signal $P^c$ and (c) calculated differential phase signal. (d) comparison of experimental and theoretical signal of the line profile indicated in (b) and (c) [96].
read-out electronics. The photon counts per physical pixel in the final image were in the order of 25000 [19]. The data was post processed with the methods explained in section 4 to resolve the fringes. The phase retrieval was done with the Hilbert transform based method (see section 5.6.3) and the sinusoidal model based method (see section 5.6.4).

Figure 8.3 shows the results of a polyethylene sphere with a diameter of 700 µm and a nylon fiber with 150 µm diameter. The absorption contrast, depicted in figure 8.3a, was retrieved with the method explained by equation 5.41. The phase signal of figure 8.3b was reconstructed with equation 5.42. Since, these materials have no high absorption coefficient the absorption image (see figure 8.3a) has low contrast. On the other side, the differential phase contrast in figure 8.3b is higher. The SNR of the phase signal is lower compared to the absorption image, since the resolution of the interpolation method is only high enough between pixels to resolve the fringe pattern, while for the absorption image the photon counts in a pixel are sufficient (i.e. no interpolation needed).

To quantitatively validate the recorded phase signal a sample on a silicon substrate was produced. Pyramids with different sizes, ranging from 50 µm up to 350 µm are edged in a silicon waver. The edged pyramids have a slope of 54.73°. The absorption and phase signal reconstructed with the Hilbert transform method are depicted in figure 8.4. The phase signal was also reconstructed with the sinusoidal model method. A close-up of this reconstruction is depicted in figure 8.5a. Note, that for the big pyramids with a diameter of 350 µm the etching process was not completed. Therefore, the top of these pyramids is flat.

The measured differential phase values were used in order to calculate the refraction angles of the detected photons and compared to the theoretical values. The etched pyramids in Si(100) have a slope of 54.73°, which means that 16.7 keV photons impinging at the edges of the pyramids will be refracted by an angle of \( \alpha = k\delta\sqrt{2} = 4.9210 \, \mu\text{rad} \), where \( k \) is the wave number and \( \delta \) the refractive index decrement for Si, which at 16.7 keV is \( 1.7639 \times 10^{-6} \) [19].

Figure 8.5a shows a close-up of the image depicted in figure 8.4b. The yellow lines mark the regions with negative slope, while the cyan lines mark regions with positive slopes. The region marked in green was considered as background, and was used to calculate the relative phase shift.

Figure 8.5b shows the standard deviation of the slope regions and the background region,
Figure 8.3: Retrieved (a) absorption and (b) differential phase contrast images with a pixel size of 25 $\mu$m for a polyethylene sphere with 700 $\mu$m diameter (left) and a nylon rod with 150 $\mu$m diameter (right) [19].

Figure 8.4: Retrieved (a) absorption and (b) differential phase contrast images with a pixel size of 25 $\mu$m for the pyramids etched in Si [19].
while scanning the width of the window by adapting $\sigma_w$. For each slope region, which are marked in figure 8.5a in yellow for the negative slopes and in cyan for the positive slopes, the average and the standard deviation are determined. It is assumed that the slope is constant, and therefore the phase shift for each pixel in the region should be equal. Therefore, it is further assumed that the pixel-to-pixel variation of the phase signal are errors introduced by the acquisition and the phase retrieval algorithm. By scanning $\sigma_w$ and observing the error, the artifacts introduced by the phase retrieval can be minimized. The noise of the retrieved phase signal is minimal at $\sigma_w = 2.2 \, \mu m$ for the slope regions and the background region. At the moment it has not been tested, if this value of $\sigma_w$ has to be adjusted for each sample, or if it is only dependent on the experimental setup. The signal of the background region is noisier than the slope regions. This is most possibly caused by impurities left from the manufacturing process of the sample.

The measured differential phase value of the slopes $\Delta \varphi$ are $0.4938 \pm 0.0869$ rad for the Hilbert transform based method [19] and $0.4843 \pm 0.0807$ rad for the sinusoidal model based method. The refractive angles can be retrieved from the phase difference by $\alpha = \Delta \varphi g_1 / 2\pi z_t$, where $z_t = 15$ cm, from the experimental data this results in $\alpha_{exp} = 4.9249 \pm 0.8664 \, \mu rad$ demonstrating that the quantitative differential phase information is well retrieved [19]. Note that the noise of the phase signal is dependent on the reconstruction algorithm. The sinusoidal model based method reduces the error compared to the Hilbert transform based method. It is assumed that further development of the phase retrieval algorithms could reduce the error further, without changing the experimental setup.
Chapter 9

Summary and Conclusions

The main idea of this thesis was to evaluate, if grating based phase contrast measurements are possible without the analyzer grating \( G_2 \) using modern low noise small pixel hybrid detectors, and to develop the necessary tools and algorithms. In addition, the existing detector hardware had to be put in operation, tested and characterized. Software to analyze the detector data had to be written, and data-sets of several terabytes had to be analyzed. The project, therefore required a broad spectrum of knowledge in electronics, computer science and physics. At the beginning, it required intensive programming of FPGAs with VHDL for the development of the firmware to operate the detectors. Once the detectors were operational, I had to gain a deep understanding of the programming languages C, C++, Matlab and Python, to perform the data analysis in a reasonable time and to discuss best practices with the software developer involved in the controlling software. It was also necessary to have a deep understanding of the analog electronics of the used detectors. Furthermore, during the project I also acquired deep knowledge in semiconductor physics and interaction of X-rays with matter. Finally, I also had to master the physics involved in phase contrast imaging, specifically refraction, the Huygens-Fresnel principle and Fourier optics in general.

The following section describes the achievements and my conclusions in all the different aspects of this project. Beginning with data processing, detector characterization and imaging experiments, and continuing with the phase contrast imaging experiments performed in this project and shown in this thesis. The last section is a brief outlook on some more and less distant suggested tasks for a successful continuation of this project.

9.1 Achieved goals

9.1.1 Characterization of MÖNCH

One of the most important detector parameter is the noise. The noise limits the energy resolution, and also the detector position resolution using interpolation. So it is very important for the methods of this thesis. MÖNCH has an extremely low noise of 31 e\(^{-}\) ENC. Therefore, it can be used for experiments, which before were only feasible with specific low noise detectors, like CCDs or MAPS. Furthermore, MÖNCH opens the possibility to build hybrid pixel detectors for low energy applications, which was not possible before. With a noise of 31 e\(^{-}\) and a discrimination limit of 5 \( \sigma \) for single photon resolution, MÖNCH is able to detect photons from 560 eV onwards. Also in terms of pixel size MÖNCH is now comparable to CCD and MAPS detectors.
Important for the position interpolation is the charge sharing behavior. It was therefore extensively studied using different methods. Specifically the edge-on experiment (see section 6.4) gives detailed insight into the depth dependence of the charge sharing. By illuminating the sensor with a collimated 20 keV beam from the side, it was possible to control the absorption depth of the photons in the sensor material. This allowed to infer that the charge sharing is highly dependent on the absorption depth in the sensor. The conclusion made from this experiment where used, to develop position interpolation algorithms presented in chapter 4. Under consideration of the charge sharing between pixels of pixelated hybrid detectors, a spectral fitting function for the signal response of a pixel is presented in section 3.3.

For this thesis the position resolution, which is dependent on the detector noise, is also important. The position resolution limits the resolution of the phase signal of the phase contrast measurement. To evaluate the position resolution of MÔNCH independent from the grating interferometer, it was measured in combination with the interpolation algorithms with a knife edge measurement (see section 6.5). It was discovered that the spatial resolution is dependent on the in-pixel position of the photon absorption event, since the amount of charge sharing changes with the in-pixel position. The average spatial resolution is between 4 \( \mu m \) and 5 \( \mu m \) for the investigated energy range, while it is as low as 3 \( \mu m \) in the best case. The influence of the angular alignment error of the detector surface normal to the incoming beam was shown mathematically in section 6.5.1.

In this thesis it is also demonstrated, that MÔNCH is a suitable detector for energy discriminating imaging (color imaging). It was possible to distinguish emission lines of materials with a distance of \( \pm 500 \) eV (see section 7.5). The noise performance of the detector, presented in section 6.2, allows to discriminate photon energies with a resolution of \( \pm 120 \) eV RMS.

9.1.2 Post processing of silicon hybrid detectors data operated in single photon regime

The advantages of operating silicon hybrid detectors in the single photon regime were carefully investigated in this thesis, in particular, the energy determination and the absorption position for each photon absorbing event. In a second step, processing software for the big amount of data was developed. The software analyzes the data in three steps. First, the photon hits are discriminated from the background noise of the detector and extracted. Second, the spatial resolution algorithm is calibrated with a blank measurement. And as a third step, the acquired sample data is analyzed and a high resolution image, with a finer resolution than the physical pixel pitch would allow, is produced. Note that, during this process of refining the position resolution for each absorption event, the photon energy information is preserved. The algorithms adapted and produced during this project are described in chapter 4.

9.1.3 Imaging capabilities of silicon hybrid detectors

In section 7.2 it is shown that MÔNCH and GOTTHARD in combination with the developed high resolution imaging algorithms are suitable instruments for imaging of medical samples. Feature sizes of microns are still resolved in good quality. Furthermore, in an experiment described in section 7.3, the capabilities of GOTTHARD as a detector for tomographic imaging were demonstrated. Standard tools for tomographic reconstruction could be used to successfully perform the Radon transform on the produced data. In combination with an x-ray microscope, it was shown that MÔNCH has a comparable performance to a water-cooled charge coupling device (see sec-
9.2 Perspectives

Hybrid pixel detectors operated in the single photon regime, in combination with the small pixel pitch and low noise performance given by MÖNCH, allow a variety of possible applications for this detector. Optimal applications are those with low flux, particularly inelastic X-ray scattering [103], where precise spectrometers are needed. Other possible applications are low energy experiments, that now are possible with a hybrid detector with such low noise.

To investigate the new possibilities further, a second prototype with a field of view of 1 cm$^2$ was already developed and tested by the SLS detector group during the write-up of this thesis. Promising experiments at the Phoenix beamline of the Swiss Light Source were already conducted with this new prototype.

Furthermore, the data processing system, coping with the huge amount of data produced by such detectors, is continuously improved, so that transparent use of the algorithms presented in chapter 4 will be possible by users in the near future.

One major limiting factor of the current MÖNCH detector is the relatively slow frame-rate of 2 kHz (8 kHz with the new prototype). Increasing the frame-rate further will allow experiment times in the same magnitude as they are common with conventional detectors, while the gained data precision is much higher in terms of energy and position. Also the high information content for each absorption event will allow to make dose-sensitive experiments more efficient, thus opening the field for medical and biological imaging.

During the development of the algorithms for this thesis, many ideas for improvements came up. One major requirement is the online processing of the output data, which will probably require a scalable software or hardware solution running on many CPUs. Another improvement would be the adaption of the position interpolation algorithm for different sensor materials like GaAs and CdTe. This requires a careful study of the charge sharing behavior in such sensor materials, but would allow to perform interpolation with hybrid detectors at X-ray energies up to 100 keV.

Omitting the need of the analyzer grating in the grating interferometer, and therefore also the stepping procedure, allows new experiments with two-dimensional gratings, where the differential phase shift signal of the sample can be recorded in two-dimensions. This allows more stable reconstruction of the phase information. Two-dimensional grating interferometry is also possible.
with an analyzer grating, but the acquisition times are very large, since the stepping procedure has to be performed in two-dimensions as well.
Bibliography


[34] Th Thüring et al. “Human hand radiography using X-ray differential phase contrast combined with dark-field imaging”. In: Skeletal radiology 42.6 (2013), p. 827.


[47] A Abboud et al. “Sub-pixel resolution of a pnCCD for X-ray white beam applications”. In: Journal of Instrumentation 8.05 (2013), P05005.


Appendix A

Curriculum vitae