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Monte Carlo and Charge Transport Simulation of Pixel Detector Systems

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Monte Carlo and Charge Transport Simulation of Pixel Detector Systems

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To my son Oliver
ABSTRACT

This thesis is about simulation of semiconductor X-ray and particle detectors. The simulation of a novel coating for solid state neutron detectors is discussed as well as the implementation of a simulation framework for hybrid pixel detectors.

Today's most common thermal neutron detectors are proportional counters, that use $^3$He gas in large tubes or multi wire arrays. Global nuclear disarmament and the increase in use for homeland security applications has created a shortage of the gas which poses a problem for neutron spallation sources that require higher resolution and larger sensors. In this thesis a novel material and clean room compatible process for neutron conversion are discussed. Simulations and fabrication have been executed and analysed in measurements. It has been proven that such a device can be fabricated and detect thermal neutrons.

Spectral imaging hybrid pixel detectors like the MEDIPIX chip are the most advanced imaging systems currently available. These chips are highly sophisticated with several hundreds of transistors per pixel to enable features like multiple thresholds for noise free photon counting measurements, spectral imaging as well as time of arrival measurements. To analyse and understand the behaviour of different sensor materials bonded to the chip and to improve development of future generations of the chip simulations are necessary. Generally, all parts of the detector system are simulated independently. However, it is favourable to have a simulation framework that is able to combine Monte Carlo particle transport, charge transport in the sensor as well as analogue and digital response of the pixel read-out electronics. This thesis aims to develop such a system that has been developed with Geant4 and analytical semiconductor and electronics models. Furthermore, it has been verified with data from measurements with several MEDIPIX and TIMEPIX sensors as well as TCAD simulations.

Results show that such a framework is feasible even for imaging simulations. It shows great promise to be able to be extended with future pixel detector designs and semiconductor materials as well as neutron converters to aim for next generation imaging devices.
SAMMANFATTNING

Avhandlingen behandlar simulering av processerna i röntgen- och partikeldetektörer från den fysiska interaktionen i sensorn till utsignalen från detektorn. Simuleringarna har gjorts med fokus på fotonräknamne hybriddetektörer för spektral avbildning. Dessutom behandlas en ny halvledarbaserad neutrondetektor.


Sammanfattning

för tillverkning av detektorer för framtidens neutronkällor.
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LIST OF PAPERS

This thesis is based on the following papers, herein referred to by their Roman numerals:

**Paper I**
Simulation of a silicon neutron detector coated with TiB$_2$ absorber

**Paper II**
A thermal neutron detector based on plana silicon sensor with TiB$_2$ coating

**Paper III**
Simulation of the Spectral Response of a Pixellated X-Ray Imaging Detector Operating in Single Photon Processing Mode

**Paper IV**
Investigation of charge collection in a CdTe-Timepix detector
D. Krapohl, E. Fröjd, D. Maneuski, H.-E. Nilsson, and G. Thungström,
Journal of Instrumentation, 2012 ................??

**Paper V**
Spectral resolution in pixel detectors with single photon processing
C. Fröjd, D. Krapohl, S. Reza, E. Fröjd, G. Thungström, B. Norlin,
Proceedings of SPIE, 2013 ................??

**Paper VI**
Fabrication, characterization and simulation of channel stop for n in p-substrate silicon pixel detectors
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Paper VII
Readout cross-talk for alpha-particle measurements in a pixelated sensor system

Paper VIII
A Geant4 based framework for pixel detector simulation

Paper IX
Verification of Geant4 pixel detector simulation framework by measurements with Medipix family detectors
D. Krapohl, A. Schübel, E. Fröjd, C. Fröjdh, and G. Thungström, Transactions on Nuclear Science, 2015 ..................
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INTRODUCTION

Radiation detectors are used for all kinds of purposes in many aspects of life. In the following sections these will be motivated for the neutron and X-ray pixel detectors separately.

1.1 Solid state neutron detectors

Neutron detectors are employed in several areas such as nuclear reactors, material science, radiation safety as well as radioactive substance detection in homeland security applications. Neutrons are not very easy to detect, their interaction properties with different materials change with energy. The main focus of the work on neutron detectors lies on the detection of thermal neutrons.

A background of high energy gamma photons creates noise in the detector that has to be discriminated. There are mainly three types of detectors, gas proportional counters, scintillation detectors like glass fibres and semiconductor detectors with converter layers. Generally, certain isotopes light atoms like hydrogen, helium as well as lithium and boron have a high capture cross section for slow or thermal neutrons. $^{235}$U (uranium) can also be used in neutron detection but undergoes nuclear fission reaction. Especially, $^3$He gas filled proportional counters are common. The helium isotope is rare and most of it is produced in the decay of tritium in nuclear weapons. In recent years there has been a shortage of the gas caused by the nuclear disarmament. Semiconductor, i.e. silicon, neutron detectors need converter layers that capture neutrons and convert them into ionizing radiation. These assemblies have the advantage that they can be integrated with amplifiers and logic elements. Their downside has been a poor detection efficiency for neutrons and eventually bad discrimination against other types of radiation. Recent advances in manufacturing techniques allow for improved geometries, for example stacking of layers, thereby improving the detection efficiency [Mcg+03]. A second prospect is the integration of these converter layers with hybrid pixel detectors such as the Medipix system allowing for high resolution neutron imaging which might be interesting for experiments at the upcoming European Spallation Source (ESS) [Lin+11].
1.2 Simulation of pixel detectors

X-ray radiation detectors are used in many areas such as medical and security applications, material science as well as in life sciences. Hereby properties like absorption after passing through matter, fluorescence or diffraction can be used to gather information about the examined specimen. In the beginning photographic plates and films were used followed by photostimulable phosphor plates (PSP) and flat panel detectors (FPD). PSPs trap charges when exposed to radiation and are read out by scanning them with a laser. The latter are in use in modern hospitals as they are more sensitive than film and therefore allow for a lower dose in patients as well as digital readout. FPD use amorphous selenium to cover large areas. The electron/hole pairs created in the selenium layer are directly read out with a thin-film transistor array. The advantage over PSP plates and scintillators is an improved resolution by excluding the dispersion of optical photons in the phosphor or scintillator. A lot of research is done on energy resolving, photon counting, hybrid pixel detectors resulting in systems like MEDIPIX and TIMEPIX, Pilatus and Eiger and HEXITEC [Llo+07; Bal+11; Brö+01; Din+11; Jon+09]. Energy resolved imaging systems offer prospects like spectral imaging and “colour”-X-ray by choosing multiple appropriate energy thresholds.

In order to characterize and understand these detectors better detailed simulation models have to be available. This knowledge is vital to design future generations of detector electronics and sensor components.
Chapter 2

METHODS

The following chapter gives an overview over the used techniques, software programs and measurement systems. In the first section two different simulation methods are explained. The following section describes the Medipix hybrid pixel detector that was used to gather data for verifying simulation models.

2.1 Simulation tools

Monte Carlo particle simulation and TCAD process and device simulation are the two main methods that have been used throughout the work of this thesis. Their principles and differences are explained in the following sections.

2.1.1 Simulation of particle interaction with matter

The Monte Carlo technique is based on using random numbers and probabilities to solve mathematical problems. The term was introduced by Metropolis and Ulam in 1949 [MU49]. In the field of physics several Monte Carlo packages of different origin are available to simulate the passage of particles through matter. MCNP was developed at the Los Alamos National Laboratory and is written in Fortran. According to the website, “MCNP is a general-purpose Monte Carlo [...] code that can be used for neutron, photon, electron, or coupled [...] transport.”

FLUKA is another Monte Carlo simulation package and the German acronym for “fluktuierende kaskade”. The software is developed in Fortran and parts of it were used in Geant3 code [Fer+91]. ROSI is developed at the University of Erlangen using several established packages from other sites to provide object oriented Monte Carlo code [GWA03]. Geant4 is a Monte Carlo Simulation framework written in C++, actively developed and verified at CERN and FERMILAB. The user writes an application based on the framework that can be extended with custom code. This flexibility led to choosing Geant4 as the main simulation framework and base for the development of Geant4Medipix [Sch+14].

1https://mcnp.lanl.gov/, 2014-09-11
2.1.2 TCAD simulation

TCAD is short for Technical Computer Aided Design but does not really explain the function. Usually, TCAD summarises software that can be used for process (clean-room processes) and semiconductor device simulations. However, it can also be used for combined thermal, optical and electrical simulations as well as combined with SPICE simulation. Most of these programs rely on finite volume or finite element solvers. In this technique a mesh is calculated inside a structure and partial differential equations are solved for every single mesh cell.

In this thesis several commercial programs have been used. Namely Synopsys MEDICI, Synopsys TCAD Sentaurus, Silvaco Atlas and Comsol. MEDICI is based on the PISCES (Poisson and Continuity Equation Solver) simulator developed at Stanford University [PRD84; RC88]. The Sentaurus tools sproces and sdevice are originally developed at the University of Florida and were called FLOOPS/FLOODS (FLorida Object Oriented Device and Process Simulator) [Law94]. Silvaco Atlas is using the same syntax as MEDICI but completely rewritten in C++. Finally, Comsol started as a collection of Matlab scripts and is a multi-physics finite element solver and has recently included a semiconductor module.

2.2 Medipix detector family

MEDIPIX is the name of a collaboration of several international universities and research institutes led by the microelectronics group at CERN. The aim is to develop future generations of photon counting hybrid pixel detectors. These detectors are based on flip-chip technology and consist of a chip that can be bump bonded to a sensor. Bonding of different sensor materials to the chip is possible and enables to combine for example high-Z semiconductors with the readout asic.

2.2.1 Medpix1

MEDIPIX1 was the fist chip of the family and is only listed for completeness. It was developed as a prototype for hybrid photon counting pixel detectors in the early 1997 with $64 \times 64$ square pixels of 170 µm size. The analogue front-end in every pixel contains a charge sensitive amplifier and a shaper with leakage
current compensation, a fine tunable threshold and a 15 bit counter [Bis+98]. The chip design allows to be bump bonded to silicon or GaAs sensors.

### 2.2.2 Medipix2 and Timepix

The successor Medipix2 was developed in the Medipix2 Collaboration. The chip has a matrix of $256 \times 256$ square pixels with a pitch of $55 \mu m$ size resulting in a total active area of about $2 cm^2$. It can be configured for electron or hole collection depending on the sensor that is bump-bonded. Two flexible thresholds allow energy window measurements or photon counting mode.

The Timepix chip evolved from the Medipix2 design to allow for spectral imaging with the ability of time-over-threshold (TOA) mode and time-of-arrival (TOA) mode as well as photon-counting. With its time-over-threshold feature, the chip is able to perform spectral imaging and give information about the energy deposited per pixel. The time-over-threshold method can be best explained by looking at the timing graph in figure 2.1. The top row of the graph shows the charge sensitive amplifier (CSA) output that is compared to a threshold (dashed line). If the amplified signal is larger than the threshold, a discriminator signal, symbolized by the dotted vertical lines, defines start and stop time of the clock signal. The number of clock cycles that fit in this time frame are a direct measure for the charge and thereby the energy that

![Timepix: ToT concept](image)

**Figure 2.1:** Time over threshold timing diagram. The output signal of the charge sensitive amplifier is compared to a threshold. A discriminator signal is then used to measure the number of clock cycles that correspond to the time the pulse is above the threshold.
was deposited in the detector. Its energy binning of the collected charges depends on the pixel clock. The TOA feature enables the detector to return the time of arrival of the charge cloud from a particle at the amplifier. Its general noise performance is improved over the first Medipix2 design.

2.2.3 Medipix3 and Medipix3RX

Like Medipix2 the chip offers 65,536 pixels with a pitch off 55 µm. Among other improvements over the Medipix2 chip it features a charge summing algorithm that can allocate a charge spread over a cluster of four pixels to a single pixel that counted the largest fraction. The chip can be flexibly programmed in different operation modes like fine pitch and spectroscopic mode, the first making use of every available pixel circuit while the latter connects every second pixel in both directions. Spectroscopic mode allows to make use of the free thresholds and counters in the unconnected pixel circuits increasing their number to eight per pixel and results in a 110 µm pixel pitch.
Chapter 3

RADIATION DETECTION

This chapter gives an overview of radiation interaction with matter and its phenomenons. The interaction of non-ionizing radiation is described as well as photons and charged particles. More specific detection methods are discussed in chapter 4.

3.1 X-rays and Gamma radiation

X-rays and gamma radiation high energy photons. Technically there is no difference even though sometimes X-rays are used for the lower and gamma photos for the higher energy range. X-rays can be produced in the lab in an X-ray tube using the effect of bremsstrahlung. Electrons from a heated filament at the cathode are accelerated in an electric field towards the target anode. The maximum energy of the electrons is defined by the accelerating voltage. At the anode the electrons lose their energy when they are stopped and emit bremsstrahlung. Additionally to this continuous spectrum, characteristic energy is also emitted when electrons remove K-shell electrons in the target material (see 3.4.1). Another source of γ-radiation are radioactive sources. These emit characteristic energies during their decay and can be used for calibration.

3.2 Neutrons

Neutrons lack electric charge and are therefore not subject to Coulomb interaction with electrons or particles in the nuclei. A neutron will continue its path through matter until it undergoes strong interaction with the nucleus. Generally, neutron radiation is referred to as ‘high-energy neutrons’, ‘fast neutrons’ and ‘slow-’ or ‘thermal neutrons’ depending on their kinetic energy. Fast neutrons scatter in matter with elastic collisions and lose their kinetic energy down to the thermal energy.

Neutrons can interact with matter by elastic scattering at the nuclei, expressed as $A(n, n)A$. Fast neutrons lose energy in this process.
Inelastic scattering is a second process that fast neutrons with energies higher than 1 MeV can undergo. It can be described as $A(n, n') A^*$. Hereby the nucleus remains in an excited state and may decay with $\gamma$-radiation.

Slow neutrons will also undergo elastic scattering but might also be captured by nuclei. After capturing a secondary particle is emitted from the nucleus. Several reactions are possible e.g. $(n, p), (n, \gamma) (n, \alpha)$. In the scope of this thesis only thermal neutrons were of interest as well as the neutron capture process [Kno00].

### 3.2.1 Neutron capture

Neutron capture is an important process used in neutron detection. It builds on the phenomenon that a neutron is captured in the nucleus of an atom which then sends out detectable radiation. In gas detectors $^3$He is often used since it provides an excellent gamma discrimination. Semiconductor detectors require a converter layer applied to them to be able to detect neutrons. Interesting choices are $^6$Li and $^{10}$B because both have large capture cross sections.

$$^6\text{Li} \rightarrow ^7\text{Li} + \alpha$$  \hspace{1cm} (3.1)  
$$^{10}\text{B} \rightarrow ^7\text{Li}^* + \alpha + \gamma (480 keV)$$ \hspace{1cm} (3.2)
The boron-10 neutron conversion process is depicted in section 3.2.1. Both
the α-particle and the lithium core can be detected in a semiconductor diode.
The excited core additionally emits γ-radiation which can also deposit its
energy in the detector. After neutron capture, 94% of the reactions (equation
3.2) leave the $^7\text{Li}$ atom in an excited state that returns to ground state by
emitting a 480 keV γ-photon. The energy of the alpha particle is 1.47 MeV.
The other 6% of the reactions result directly in a non-excited state of $^7\text{Li}$ with
an α-particle of 1.78 MeV (see equation 3.1) [Knooo].

![Figure 3.2: Alpha particle conversion in $^{10}\text{B}$](image)

### 3.3 Alpha particles

Charged particles interact strongly with the electrons and nuclei in matter
due to the electromagnetic force. Until it is stopped, the particle will transfer
a part of its energy to electrons and nuclei in elastic collisions leaving behind
a path of excited atoms and free electrons. Unless the penetrating particle
is a heavy charged ion its mass is small compared to the nuclei in matter.
Therefore, only a small fraction of the energy is transferred but the particle
direction can change. Collisions with electrons have the opposite effect. A
lot of energy is transferred while the direction of the impact particle is only
slightly altered. This is described in the Bethe-Bloch equation:

$$-\frac{dE}{dx} = \frac{4\pi e^4 z^2}{m_0 v^2} N_A Z \left[ \ln \frac{2m_0 v^2}{I} - \ln(1 - \beta^2) - \beta^2 \right]$$  \hspace{1cm} (3.3)

with $\beta$ defined as

$$\beta = \frac{v}{c}$$  \hspace{1cm} (3.4)
where $c$ describes the speed of light and $v$ the particle speed. The equation defines the energy loss $E$ over the range $dx$ in a material with a mean excitation potential $I = 237eV$ for silicon. $N_A$ is Avogadro's constant, $Z$ the atomic number, $m_0$ and $e$ the electron mass respective its charge and $z$ the charge of the incoming particle. The energy loss when passing through matter described with $\frac{dE}{dx}$ is called Bragg curve. The energy deposit along a track increases towards the end and results in the so called Bragg peak [Knooo].

### 3.4 Interaction of photons in matter

Unlike charged particles that interact with nuclei or electrons along its path photons penetrate until they interact with one atom. There are three effects that are important for particle detection: the photoelectric effect, the Compton effect and pair-production. The sum of the attenuation for these three effect can be expressed as

$$I(x) = I_0 e^{-x\mu}$$

with the intensity $I_0$ and the attenuation coefficient $\mu$.

![Attenuation in CdTe](image)

*Figure 3.3: Attenuation in silicon an CdTe from $1 \times 10^{-3}$ MeV to $1 \times 10^3$ MeV*

#### 3.4.1 Photoelectric effect

If the incoming photon vanishes after interacting with an atom, the process is called photoelectric effect. All its energy is transferred to an electron of
the atom minus its binding energy. This electron can either be elevated to a higher energy level in the electron shell of the atom or become a free electron. For sufficiently large energies the photon is most likely to interact with a K-shell electron. The electron vacancy is filled by reorganization of the other electrons in the outer shell and the excess-energy is emitted as characteristic X-ray also called fluorescence. With increasing energy of a photon, the cross section (the scattering probability) of the photo, decreases. This leads to an abrupt increase of the cross section when the energy needed for freeing an inner electron is exceeded and is called k-edge (see figure 3.3). Furthermore, the cross section depends strongly on the atomic number of an element (with $Z^{4-5}$) which makes high-Z materials interesting for sensor development intended for high energy X-rays [Kno00; Tav10].

3.4.2 Compton effect

Elastic collisions between photons and electrons of the outer shell of an atom are called the Compton effect. A fraction of the photon energy is hereby transferred to the electron that is ejected from the atom at an angle $\phi$ and the photons trajectory is changed at an angle $\theta$ as depicted in figure 3.4b.

![Sketch showing the processes of the photoelectric effect (a) and Compton effect (b).](image)

The photon energy can be written as $\hbar \omega$ and its impulse momentum is $\hbar \omega / c$. Keeping in mind that energy and momentum has to be conserved, the
Chapter 3. Radiation detection

The following expression can be used for the energy of the recoil electron:

\[ E' = h\omega' = \frac{h\omega}{1 + \frac{h\omega}{m_e c^2} (1 - \cos \theta)} \quad (3.5) \]

with scattering angle of the photon \( \theta \), and electron mass \( m_e \). The equation has a maximum at a scattering angle of 180° [Tav10].

3.4.3 Pair production

Pair production occurs with increasing probability for higher photon energies (exceeding an energy of 1.022 MeV which corresponds to \( 2m_e c^2 \)). The energy of a photon is thereby used to create a positron-electron pair:

\[ \gamma \rightarrow e^+ + e^- \quad (3.6) \]

The created positron is usually quickly annihilated creating two photons with an energy of 511 MeV each leaving in opposite directions [Kno00].
In this chapter particle detection methods and commonly used systems are described. The first section gives an overview over different types of detectors. Neutron detection in particular and semiconductors are discussed in the following.

This chapter gives an overview of semiconductor materials and detector design. Important properties such as charge transport and signal formation in planar and pixel detectors are discussed as well as degrading factors in pixel devices.

### 4.1 Semiconductors

Nearly all electronic devices and silicon detectors rely on a pn-junction. However, a pn-junction is not necessarily required for radiation detection in a semiconductor. The most important semiconductor materials are silicon and germanium. In the recent past manufacturing processes have improved the quality of compound semiconductors so that materials like gallium-nitride, cadmium-telluride and cadmium-zinc-telluride are of growing interest for detectors. These high-Z materials are often used with high resistivity and ohmic contacts.

Silicon has four valence electrons, two of them in the 3s and two in the 3p orbital. In a crystal these 4 electrons are shared in the bonds between atoms. Silicon crystallizes in the same configuration as diamond with parameters like electron drift velocity depending on the crystal direction. Atoms in a crystal arrangement appear as energy bands that depend on the lattice direction with a region between called band-gap. The valence electrons build up the valence band. Any higher electron level is called conduction band. The energy of the band-gap defines if a material is a conductor, a semiconductor or an insulator, i.e., conduction and valence band are overlapping, the band-gap has a low energy or a high energy gap.
4.1.1 PN-junction

If donor atoms from group III or V in the periodic table are introduced into the silicon lattice, the crystal becomes either p-type or n-type. Placing a p-region and an n-region adjacent to each other results in a pn-junction. This is illustrated in figure 4.2 and presents a diode. Both sides are electrically neutral. Due to the introduction of foreign atoms, the p-type region has many holes in the valence band and very few electrons in the conduction band and vice versa in the n-type part of the structure. These free charges will build up a potential after drifting to opposite sites of the device. This built-in potential, however, is not directly measurable because of the contact potential between silicon and a metal.

In the device a so called depletion region forms with a built-in potential of around 0.7 V (see figure 4.2). This can be estimated with

$$V_b \approx \frac{kT}{q} \ln \left( \frac{N_D N_A}{n_i^2} \right)$$  \hspace{1cm} (4.1)

when full ionisation of donors and acceptors is assumed. $V_b$ is the build in potential, $k$ Boltzmann's constant, $T$ the lattice temperature, and $q$ the electron charge. In the bracket $N_D$ and $N_A$ describe the donor and acceptor density, respectively, as well as the intrinsic number of charge carriers $n_i$. 

Figure 4.1: Band diagram of silicon. The bands drawn in red belong to the conduction band and the bands in blue belong to the valence band.
4.1.2 Electric field

The depletion region can be expanded by applying an external reverse bias voltage to the contact causing first full depletion and later over-depletion of the device. The extent of the depletion region is then described by

$$W = \sqrt{\frac{2\varepsilon_0\varepsilon_{Si}}{q} \left( \frac{1}{N_A} + \frac{1}{N_D} \right) (V + V_b)},$$  \hspace{1cm} (4.2)

where $W$ is the length of the depletion width extending into both n- and p-region, and $V$ the externally applied voltage. Without reverse bias the depletion width is about 1 µm for the simulated device shown in figure 4.2. An external voltage will extend the depletion region over the whole structure. Increasing the external bias voltage further will result in avalanche breakdown.

The voltage that is required to expand the depletion zone over the entire thickness of the sensor volume can be described as:

$$V_{depl} = \frac{qN_Dd^2}{2\varepsilon_0\varepsilon_{Si}}$$  \hspace{1cm} (4.3)
with $N_D$ the donor concentration, the thickness $d$, $\varepsilon_{Si}$ the relative permittivity of silicon.

As mentioned before, a pn-junction is not required to build a working detector. High resistivity materials like CdTe and CZT are often used with ohmic contacts to build detectors. The electric field inside such a detector is constant throughout the whole structure just like that of a parallel plate capacitor.

### 4.2 Charge transport

The two most important phenomena in a semiconductor detector with free carriers and an electric field are drift and charge diffusion.

#### 4.2.1 Diffusion of charge carriers

Diffusion is the effect of a high concentration of charge carriers spreading towards the region with lower concentration. The current caused by charge diffusion can be described in

\[
J_{n,\text{diff}} = -D_n \nabla n = -\frac{kT}{q} \mu_n \nabla n
\]

\[
J_{p,\text{diff}} = -D_p \nabla p = -\frac{kT}{q} \mu_p \nabla p
\]

with $\nabla n$ and $\nabla p$ the gradients of electron and hole concentration respectively. $D$ is the diffusion constant describing the random motion of charge carriers.

\[
D_{n,p} = \frac{\mu_{n,p} k_B T}{q}
\]

with $\mu$ the mobility, $k_B$ Boltzmann's constant and $T$ the absolute temperature.

#### 4.2.2 Drift of charge carriers

A charged particle in an electric field begins to drift along the field lines. In the semiconductor lattice, the moving particle will randomly scatter. Its average velocity $v$ can then be described by

\[
v_n = -\mu_n E
\]

\[
v_p = \mu_p E
\]
4.2.2. Drift of charge carriers

with $v_n$ for electrons and $v_p$ for holes with their respective mobility $\mu_p/h$. In a stronger electric field the number of collisions in the lattice increases compensating the effect of stronger acceleration which leads to a saturation of the drift velocity [Jac+77]:

$$\mu = \frac{v_s/E_c}{\left[1 + (E/E_c)^\beta\right]^{1/\beta}}$$  \hspace{1cm} (4.9)

![Field dependent mobility](image)

**Figure 4.3:** Field dependent mobility fitted with parameters from Jacoboni et al. [Jac+77]

The intrinsic mobility of silicon at room temperature (300 K) is about

$$\mu_{0,n} = 1400 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$$  \hspace{1cm} (4.10)
$$\mu_{0,p} = 480 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$$  \hspace{1cm} (4.11)

with $\mu_o$ the mobility for electrons (n) and holes (p). Moving charge carriers cause a drift current that can be expressed as

$$J_n = -q\mu_n E$$  \hspace{1cm} (4.12)
$$J_p = q\mu_p E$$  \hspace{1cm} (4.13)

with $J_{n,p}$ the current density in A cm$^{-2}$.  

page | 17
4.2.3 Shockley-Ramo theorem and signal formation

A charge (electron/hole pairs) $q$ from an energy deposition of a photon or charged particle starts to move along the field lines of the electric field in the detector. This movement instantaneously induces a current at the electrodes corresponding to the deposited energy. It is not the charge cloud that arrives at the electrodes of the detector that defines the signal. The induced current $i$ at the electrodes of a planar device is defined by:

$$i = qvE_0$$ (4.14)

Figure 4.4: Weighting potential for a planar structure (electrode with infinite length) on the left and weighting potentials for 55 µm and 110 µm pixel pitch.

with the electron charge $q$, the weighting field $E_0$ and the velocity $v$. For a pixel detector the signal formation is slightly more complicated. It can be expressed as a weighting potential. The weighting potential does not correspond to the electric field of the detector, but can be obtained by setting one electrode to unity potential while all others are at 0 V; the electric potential shows the distribution of the weighting field. A plot of the weighting potential for a planar device and two pixel sizes can be seen in figure 4.4.

The integration of the induced current over time equals the charge $Q$:

$$Q = \int_{t_1}^{t_2} i(t) dt = q \left[ \phi_0(x_1) - \phi_0(x_2) \right]$$ (4.15)
4.2.3. Shockley-Ramo theorem and signal formation

which corresponds to the elementary charge multiplied by the difference in the weighting potential at the positions $x_1$ and $x_2$ at time $t_1$ and $t_2$. For a planar device this charge is the same for any equally long drift path, that is, electrons and holes drifting from the centre of the device to opposite electrodes induce the same amount of charge if none of them recombine.

Figure 4.5: Sketch of a hybrid pixel detector. The chip contains amplifiers and pixel logic as well as controlling periphery. Solder bumps are placed on the bump pads on the chip and pressed against their counterpart on the sensor.

In a pixel detector with electrode contacts much smaller than the device thickness, the weighting potential becomes denser closer to the electrode. The smaller the contacts are that define the pixels the closer the weighting potential lines move towards it so that a larger part of the structure has nearly no influence on the induced signal. That means most of the signal is induced by charges moving close to the electrode. Hence, very little signal is induced by a moving charge cloud far from the electrode (see 4.4 plot 2 and 3). Therefore, charges drifting to the backplane of the device do not significantly contribute to the signal unless their origin was close to the electrode contact. This effect is in particular useful for materials that are prone to charge trapping and/or exhibit bad hole mobility, if electrons are collected, that is.

As a consequence of the weighting potential lines extending onion-peel-like from the contact, signal is also induced in the neighbour pixels but the sign of the induced current is reversed when a moving charge comes close to the pixel.
4.3 Pixel detectors

Radiation images can be obtained in different ways, with films charge integrating devices and single photon counting detectors. Digital systems have the advantage that information can be read and displayed in real-time.

CCDs and CMOS sensors are examples of charge integrating devices. The circuit structures for amplification and digitization sit along the periphery and are embedded together with the photo diode in the same semiconductor structure. Their advantages are high spatial resolution and low production costs with the drawbacks of integration of noise and leakage current.

Single photon counting detectors contain electrical circuits in every pixel which allows to suppress electronic readout noise directly in the pixel. Figure 4.6 shows a cross section through a single pixel of a hybrid pixel detector where the sensor material is connected to the electronics chip via a solder bump.

Electron hole pairs generated by radiation drift in an electric field towards the electrode and are collected. The current signal from the sensor is amplified in the pixel electronics, compared to a threshold and digitized. The sensor matrix is flip-chip bonded to the readout chip that is mounted on a PCB where wire bonds connect the chip to the read-out electronics (see figure4.5). The analogue and digital circuitry can also be embedded in the sensor to form a monolithic chip.

However, a big advantage of a hybrid pixel detector is that it allows to combine the amplification and digitization electronics on one chip with other sensor materials than silicon, e.g. CdTe, CZT or GaAs [Ros+06].
4.4 Charge sharing

The term charge sharing is usually used in the context of particle interaction in the sensor, e.g. the direction of the particle track, fluorescence photons, secondary electrons, and diffusion processes (see figure 4.7), but can also be caused by a magnetic field perpendicular to the drift direction of the charges in the sensor.

Spatial resolution in a pixel detector can be improved by arranging pixels in a brick or hexagonal pattern. The effective pixel pitch is halved as well as the inter-pixel capacitance in one direction. Thus, every pixel can only have three neighbours at its corners which reduces the amount of 4-pixel-clusters. Yet this method is practically never used as it requires more complicated image processing algorithms. Figure 4.7 shows another source of performance degradation. Depending on where photons or ionizing radiation deposit their energy the charge can be shared by several pixels, so-called clusters. In spectral imaging this leads to lower counts per pixel as expected. A second phenomenon is X-ray fluorescence in the sensor material. If the energy of photons is higher than the K-edge energy of the semiconductor material, fluorescence photons can be emitted and might travel longer than a pixel distance. This leads to “false” counts in neighbour pixels and lower energy deposited in the pixel of the first interaction. However, this phenomenon is

---

Figure 4.7: Spatial and energy resolution is influenced by the amount of charge shared between pixels either due to diffusion or fluorescence.
more relevant in high-Z materials.

4.5 Noise performance and cross talk

There are several capacitances in a pixel detector that influence the noise performance and cross talk between the pixels:

- sensor capacitance
- sum of capacitances to the neighbours
- capacitance to ground of the readout pcb
- other contributions (bumps)
- cross talk in the chip
- Fano factor

4.5.1 Pixel capacitance

Several effects in a pixel detector can have influence on the noise performance and therefore energy and spatial resolution. Figure 4.8 shows the different capacitances that might be present in a pixel detector. The capacitance to the back plane, the sensor capacitance, behaves like a parallel plate capacitor:

$$C_j = \varepsilon_0 \varepsilon_{Si} \frac{A_{\text{pixel}}}{d} = \varepsilon_0 \varepsilon_{Si} \frac{A_{\text{pixel}}}{W}$$ (4.16)

with $A$ the area of the pixel and $d$ the thickness of the sensor or $W$ the depletion width. Therefore, $C_j$ can be described as:

$$C_j = A \sqrt{\frac{\varepsilon q N}{2 (V_r + V_b)}}$$ (4.17)

with the electron charge $q$, the doping concentration $N$, build-in potential $V_b$ and reverse bias $V_r$. The inter-pixel capacitance is a compound of the sum of the four direct neighbours and the sum of the four diagonal neighbours. The p+ implants in a p-in-n detector, which is the most usual type, can hereby be regarded as parallel wires:

$$C_{ip} = 4 C_{\text{diag}} + \frac{4 \pi \varepsilon_0 \varepsilon_r L}{\ln \left(\frac{\frac{g}{d}}{\sqrt{\left(\frac{g}{d}\right)^2 - 1}}\right)}$$ (4.18)
4.5.2 Cross talk in the chip

Another source for signal distortion is cross talk in the readout chip from digital to analogue signal lines. A voltage step can insert a charge through a parasitic capacitance in the chip. Another source can be voltage spikes in the power or bias lines. It can only be avoided by careful routing of the layout.

4.5.3 Fano factor

In a semiconductor the number of electron-hole pairs generated from energy absorption equals the deposited energy divided by the energy that is needed to create electron-hole pairs. For silicon and CdTe the factors are 3.6 eV and 4.35 eV, respectively. However, a small amount of energy is used for electron-hole separation so that the exact number of electron-hole pairs fluctuates. This can be expressed in

\[ \Delta N^2 = F \frac{E}{w} \]
where $N$ describes the number of electron hole pairs, $F$ the Fano factor, $E$ the absorbed energy and $w$ the energy required to create one electron-hole pair. The Fano factor is about 0.1 for most semiconductors and varies slightly with temperature and energy of the absorbed particle. It is an intrinsic limit for the energy resolution of the detector material.
Chapter 5

NEUTRON DETECTOR

Semiconductor neutron detectors have to rely on a converter layer that captures neutrons and converts them into ionizing radiation. Another important requirement is the ability to discriminate the events from a γ-background.

In this chapter a semiconductor neutron detector based on a new converter material is described. The design and simulation are discussed in the first two sections followed by manufacturing and measurement results.

5.1 Neutron detection

Neutrons can only be indirectly detected since they do not ionize atoms directly. However, they can be absorbed in the nucleus and spawn nuclear reactions. The most widespread neutron detectors are gas detectors using $^3$He as a converter because of its high absorption cross section and very good γ-discrimination. Eventually some other gases for gain are also added. A neutron reacts with a $^3$He atom. The reaction results in a tritium particle and a proton that drift through an electric field inside the gas chamber until collected at an electrode wire. The simplest form of such a detector consists of a tube with a central wire that is filled with $^3$He and some other gas for gain and stopping of the proton and triton particle. An electric field is applied between wire and inside of the tube. Such systems are called linear proportional counters and can be 1 m long with a resolution of 5 mm to 10 mm. Two dimensional panel shaped systems are called multi wire proportional counters (MWPC). Several wires are arranged in a cross pattern, which allows to read out current pulses in two directions, offering a resolution of 0.5 mm to 2 mm [Rad12; Kn000; CB91].

Due to the shortage of $^3$He, and higher demands on resolution semiconductor detectors are of growing interest [Kou09]. In semiconductor devices a converter layer is applied to for example a silicon diode. Neutrons are captured by the active element in the converter layer and energetic particles such as α-particles or photons are emitted. They in turn create electron/hole pairs in the semiconductor lattice. The cross section of the neutron capturing isotope should be large allowing the optimisation of the geometry of the device. Interesting candidates are $^6$Li and $^{10}$B but $^{157}$Gd and $^{113}$Cd are also isotopes
Chapter 5. Neutron Detector

with high neutron cross sections. One possibility to improve the effectiveness of such converters is to enrich its isotropic abundance, another to optimise the geometry, for example by applying several layers or 3D columns [Mcg+03]. Furthermore, the device should be able to discriminate the α-particles against γ-radiation [Kra+12].

5.2 Semiconductor neutron detector

Titanium diboride (TiB$_2$) is an interesting candidate for a converter material. TiB$_2$ is a very hard ceramic material with a density of 4.5 g cm$^{-3}$, a high melting point and a good electrical conductivity (for a ceramic material) of $1 \times 10^5$ S cm$^{-1}$ [Mun00]. The reason for choosing TiB$_2$ as a conversion material was because it can be handled by standard clean room techniques such as electron beam evaporation or sputtering despite its high melting point. Its relatively low resistance allows for layering the material on top of a device without negative impact on the signal or bias voltage that is needed to extract electron/hole pairs. Titanium is nearly transparent to slow neutrons whereas B-10, with a natural abundance of 19.8%, captures and converts them with a thermal neutron cross section of 3849 b [Knooo]. Figure 5.1 sketches the structure of the device. The titanium layer underneath the converter improves adhesion and removes stress in the diode which in turn leads to a lower leakage current. Aluminium contacts are deposited on anode and cathode of the device. The device itself consists of a silicon diode with a thin silicon epitaxial layer which is added to limit the depletion region. The idea is to reduce the number of detected gamma photons in the device.

Figure 5.1: Neutron detector fabricated by evaporating different layers on a silicon photodiode.
5.2.1 Monte Carlo simulation in Geant4

The simulated detector volume corresponds to a size of $5 \times 5 \times 0.05 \text{ mm}^3$ consisting of a silicon diode and several metal layers. The world volume surrounding the detector was a cube of the size $100 \text{ mm} \times 100 \text{ mm} \times 100 \text{ mm}$. The particle source was placed along the $x$-axis about $5 \text{ mm}$ above the device. The materials used in the simulation were defined using the NIST material database that provides the correct isotopic composition of elements [Boh05].

In a first run, the thickness of a single TiB$_2$ layer on silicon was varied between $500 \text{ Å}$ to $20 \text{ 000 Å}$ to get an understanding of its detection efficiency. This procedure was repeated with all layers of the device, i.e. a titanium coating of $500 \text{ Å}$ and a $3000 \text{ Å}$ contact layer with the TiB$_2$ sandwiched in between as shown in figure 5.1. Similar work studying boron clusters has been conducted by Guardiola et.al. [Gua+10]. The left graph of figure 5.2 shows a comparison between a direct layer of TiB$_2$ versus all layers on a diode. It can be seen that the deposition of an additional titanium layer has very little impact on the number of alpha particles detected. The right graph in figure 5.2 shows a comparison of energy deposition in two devices without the converter layer. It becomes clear that a device with an epi-layer of silicon absorbs less energy from $\gamma$-photons than diode with $500 \mu\text{m}$ thickness.

Finally, a TiB$_2$ layer thickness of $2000 \text{ Å}$ was selected for all following simulations due to manufacturing reasons, i.e. can be evaporated in a reasonable amount of time. Each simulation was run using $30 \times 10^6$ neutrons. Since

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure5_2.png}
\caption{On the left, $\alpha$ particle counts in different converter thickness of a single layer and all metal layers on silicon diode. The right graph shows a comparison of energy deposition between 500 $\mu\text{m}$ and 50 $\mu\text{m}$ thick active layers.}
\end{figure}
measurements of the manufactured device were executed with a laboratory Am-Be neutron source, which emits neutrons as well as $\gamma$-photons; it was important to simulate the response of the device to gamma photons. The neutron source contains a capsule with $^{241}$Am(Americium) emitting $\alpha$-radiation of which some are captured by beryllium atoms and converted to neutrons according to process described in process 5.2.

![Figure 5.3: Comparison between three different versions of the neutron detector. 500 µm device and 50 µm active layer front and back illuminated.](image)

The excited $^{237}$Np* atom de-excites with a probability of 42 % and 35.9 % with gamma photons carrying the energies $E_{\gamma 1} = 13.7 \text{ keV}$ and $E_{\gamma 2} = 59.5 \text{ keV}$, respectively. The de-excitation energy of $^{12}$C* is $E_{\gamma} = 4.44 \text{ MeV}$ in 59 % of the decays. To create a detailed model of the neutron source, simulations were run with a number of neutrons and the corresponding amount of $\gamma$-photons and their energies. Only the first decay process of the decay chain of americium-241 was considered as well as the described $\text{B}(\alpha, \text{n})\text{C}$ reaction. In measurements, the $\gamma$-background would be considerably higher due to ageing of the americium source that produces more and more unstable elements that also emit gamma photons. These were not considered in the simulation.

Throughout all simulations only thermal neutrons with an energy of 0.025 eV were used.
5.3 Clean-room processing

As mentioned before, the described solid state neutron detector is fully clean room process compatible. The final version of the silicon diode used for $\alpha$-detection is fabricated on a low resistive wafer with 300 $\mu$m thickness and an epitaxial layer of about 50 $\mu$m. The background doping in the epitaxial layer is about $1 \times 10^{14}$ cm$^{-3}$ resulting in a resistivity of $40 \ \Omega$ cm$^{-2}$.

Electron beam physical vapour deposition (EV-PVD), a standard technique in semiconductor processing, was used to evaporate and deposit the materials on the diode. The top contact, where the converter layer is deposited, consists of three layers. First a titanium layer to provide an ohmic contact as well as stress reduction since the TiB$_2$ is a ceramic material with different expansion coefficient. TiB$_2$ is prone to flake off from the surface. Therefore, a final layer of 3000 Å was added to keep the converter layer in place and provide better adhesion for the front side contact and wire bonds.

5.4 Measurements

The laboratory neutron source is sketched in figure 5.4. It consists of a steel container lined with neutron absorber. The AmBe capsule is located in the centre of the device behind a moderator that slows down the emitted neutrons. The source has a relatively low neutron flux stated in in table 5.1. Its activity was measured with two bubble dosimeters (Bubble Technology Industries).
that contain a superheated fluid in which bubbles appear at thermal neutron exposure. The dosimeter is insusceptible to γ-photons and provides an isotropic angular response. After 15 min exposure the two devices yielded an average of 386.5 bubbles that correspond to 138 µSv which in turn corresponds to a neutron flux of 414.5 n/cm²/s.

The readout system, which was used with the neutron detector, was calibrated with alpha particle emissions from $^{239}$Pu, $^{241}$Am and $^{244}$Cm with energies of 5.155 MeV, 5.485 MeV and 5.804 MeV, respectively.

Moreover, the device was exposed to the neutron source at the Czech Metrology Institute (CMI) in Prague that provides a much higher flux. Measurements were executed by Tomáš Slaviček. The CMI source has a much higher flux of $3.25 \times 10^5$ n/cm²/s. Both devices without and with converter layer were tested and confirmed the simulation results.

![Figure 5.5: Neutron conversion spectrum measured with a laboratory AmBe neutron source.](image-url)

The neutron detection efficiency was calculated using equation (5.3). With 0.01 % efficiency obtained in the measurement, the number agrees very well with the simulation result of 0.0125 %. The efficiency of the detector can be increased when it is back-illuminated as shown in figure 5.3.

$$\eta = \frac{N}{\phi At} \cdot 100 \% \quad (5.3)$$
5.5. Detector degradation

Table 5.1: Neutron flux for all neutron sources used to test the device.

<table>
<thead>
<tr>
<th>Source</th>
<th>Flux $\phi$ [cm$^{-2}$ s$^{-1}$]</th>
<th>Neutrons</th>
<th>Time [s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>AmBe</td>
<td>$3.26 \times 10^4$</td>
<td>55969</td>
<td>66680</td>
</tr>
<tr>
<td>CMI</td>
<td>414.4</td>
<td>1706</td>
<td>54960</td>
</tr>
</tbody>
</table>

5.5 Detector degradation

The simulation showed indications of nuclear transmutation. Transmutation describes a process where a neutron is captured in the nucleus and changed into a proton and an electron. Even though $^{30}\text{Si}$ has a very small neutron capture cross section, in a high neutron flux a fraction of neutrons will be captured.

\[
^{30}\text{Si}(n,\gamma)^{31}\text{P} + \beta^{-}
\]

(5.4)

Silicon atoms are hereby transmutated to phosphorus atoms[HS76]. Long term exposure to neutrons will introduce increasing concentrations of $^{31}\text{P}$ which acts as n-dopant. This will change the electrical behaviour of the device, i.e. the pn-junction deteriorates.
PIXEL DETECTOR SIMULATION

The following chapter discusses a method to combine Monte Carlo and finite element semiconductor simulation (TCAD). In the first section the simulation flow is described with the configuration of Geant4 as well as the construction of the CdTe model in MEDICI.

6.1 Geant4 and TCAD Medici

In a first approach to model processes in the sensor material of pixel detectors, a Timepix chip with a 1 mm Cadmium-Telluride (CdTe) sensor, particle stopping was modelled with Monte Carlo software and the charge-carrier drift and diffusion with TCAD software. The deposited energy obtained in Geant4 was transferred into electron/hole pairs and after a coordinate system transformation inserted into Synopsys Taurus MEDICI as photogeneration [Autio].

![Flow chart](image)

Figure 6.1: The flow chart shows the approach to simulate a full spectrum with a coupled simulation of Geant4 and MEDICI.

6.1.1 Monte Carlo simulation configuration

A slab of CdTe with the dimensions 10 mm×10 mm×1 mm was configured in Geant4 9.3p1 with material parameters from Sadao [Sad07]; Strauss [Str77]. The Livermore model for low energy physics was enabled as well as Compton scattering, photoelectric effect and fluorescence. The simulation parameters for Geant4 were specified in a macro file with 500 events. Events that had
Chapter 6. Pixel detector simulation

their final state in a volume of 220 µm × 55 µm × 1 × 10^4 µm, corresponding to one row of four pixels, were selected and their energy converted to a charge density with a conversion factor of 4.43 eV. The coordinates were transformed from (x, y, z) to (x, y)-format since MEDICI runs a 2D simulation with a standard thickness of 1 µm. MEDICI has an upper limit of two simultaneous charge depositions that can be tracked. This required to split the energy depositions into several simulation files such that each contained one charge cloud.

![Image](Figure 6.2: Simulation 3d-2d and pseudo 3d)

6.1.2 TCAD drift diffusion simulation

As mentioned before MEDICI was used to implement the charge transport simulation. The simulated volume had a size of 220 µm × 1 µm × 1 × 10^4 µm with five ohmic contacts defined on one side and one large contact covering the other side. The three contacts in the centre were 55 µm wide while the other two on the edge were smaller to keep the number of mesh elements low. The finite element models of HgCdTe present in MEDICI was adapted to CdTe. Hole and electron mobility was set to 75 cm^2 V^{-1} s^{-1} and 1050 cm^2 V^{-1} s^{-1} respectively. The resistivity of cadmium-telluride was adjusted to 1 × 10^8 Ω cm according to a doping compensation model published by Fiederle et al. [Fie+98]. The materials relative dielectric constant ε_r to 10.9 [Ada07].

Each charge density cloud from the original energy deposition in Geant4 was written to a separate input file for MEDICI. That means that, depositions from fluorescence or Compton scattering were tracked separately and then set back together with the help of the event number of their parent particle
6.1.2. TCAD drift diffusion simulation

Figure 6.3: The figure shows drifting charge carriers with an equivalent energy of 25 keV in a 1 mm thick CdTe sensor with an initial placement at the centre. Contacts are shown in pink.

used in Geant4. Electrons and holes drift in the electric field and induce a current at the pixel contacts which was integrated over time to obtain the corresponding charge.

In figure 6.3 different time steps of the transient part of the MEDICI simulation are depicted. The structure shows is 400 µm wide and 1000 µm high. Contacts are shown in pink color. The colour range shows the hole and electron densities in the material drifting towards anode and cathode. In CdTe the hole mobility is much lower than the electron mobility which can be seen in figure 6.3. Electrons are quickly collected at the pixel electrodes on top while the holes are still moving towards the back plane.

For 20 keV and 40 keV photons, the results are shown in figures 6.4 and 6.5. Each of the spectra contains energy depositions from about 500 photons simulated in Geant4 and at least as many simulation runs in MEDICI (more for long range fluorescence). For higher energies it becomes clear that this approach poses difficulties, only after summing the current in three centre electrodes, the photo peak becomes clearly visible. This is because the second energy being above the K-edges of cadmium and tellurium (26.727 keV and 31.817 keV). These photons have a range reaching into the neighbour pixels worsening the energy resolution. Another cause for error is the fact that all charge is squeezed in a 1 µm slice in Medici which does not give a realistic
Figure 6.4: Spectrum 20 keV showing the energy deposition for all single pixels and the summed spectrum.

Figure 6.5: Spectrum 40 keV photons showing the energy deposition for all single pixels and the summed spectrum.

approach was tested. Instead of neglecting the z-component in space (Geant4 coordinate system) and placing all deposition from a single event into one slice, the z-coordinate was translated into independent MEDICIsimulations and later combined. This slicing is depicted in section 6.1 on the right side. This increases the amount of finite volume simulations that have to be com-
puted but was believed to have a closer resemblance to reality in terms of charge densities with the disadvantage of repeating the weighting potential of the middle slice through a pixel. The fact that only the centre cross section of the weighting potential is used in all simulations might be the cause for the overestimation of energy in all obtained spectra.

3D simulations in TCAD Sentaurus sdevice are possible but not feasible for many photons that are required for a spectrum as they would require extreme amounts of time to run.

Figure 6.6: Spectrum for 60 keV photons showing the summed spectrum.
GEANT4 AND CHARGE TRACKING

With the experiences and difficulties from chained Monte Carlo and TCAD simulations, many parts of the procedure could be improved. At higher energies it became increasingly difficult to get an accurate picture of what happens in the sensor. There was also no room for charge processing algorithms since spatial information in one direction is missing or only possible to obtain with complex scripting schemes.

The extension to Geant4 makes it possible to cut out several steps of data conversion between Monte Carlo simulation and charge tracking simulation. Additionally, the whole detector chain can be simulated in one run from particle interaction with matter over charge drift and induction to the charge sensitive amplifier as well as digital algorithms.

7.1 Simulation program structure

The addition to Geant4 to enable charge tracking and amplifier behaviour is modularly structured and called Geant4Medipix. The Geant4 extension uses the standard Geant4 macro file format to configure simulations as well as an additional ini-file that contains material properties and standard chip settings. These values influence the settings in the DetectorConstruction class. The same file contains also the geometry settings in standard Geant4 format. Additionally, it is possible to read CAD geometries using the cadmesh library [Poo+12]. A program run can contain several events, the number of particles simulated. Every event that produces secondary particles or energy deposition in the sensor creates a HitList that contains information about the interaction. It contains information about the interaction point, the energy, pixel position, which event created the interaction and the interaction time (see figure 7.1). The HitList is transferred to the Digitizer which is responsible for the electron/hole cloud tracking in the electric field. The output is transferred to the Preamplifier. The last step emulates the logic of the digital part of the chip.
Chapter 7. Geant4 and charge tracking

Figure 7.1: The simulation is configured with two files. The ini-file contains fixed parameters like material properties and the mac file controls the simulation run.

7.2 Geometry

Figure 7.2 shows a typical geometry of a sensor with 10×10 pixels and their bump bonds. Any kind of combination of pixel size, sensor thickness and number of pixels can be configured. In Geant4 the geometry is placed inside a world volume. The pixel matrix is constructed by replicating one prototype which simplifies creating complex sensor geometries as well as keeps a low memory footprint. Figure 7.2 shows an example of 10×10 pixels arranged in a sensor with 300 µm height and bump bonds enabled as a wire frame model. The geometry of the chip and printed circuit board is disabled for better visibility.

Figure 7.2: 300 µm sensor with pixel volumes and bump on top arranged in a 10×10 matrix.
7.3 Digitizer

The Digitizer processes the *Hitlist* which is sent for every event interaction. Based on this information it processes the hits and outputs the induced current at the pixel electrode (see figure 7.1 and figure 7.4). The charge depositions of secondary particles of an interaction are treated as independent events without interaction between them. This simplification is used due to the charge tracking algorithm.

![Digitizer diagram]

- **Digitizer:**
  - tracking e/h pairs in E-Field
  - drift/diffusion/repulsion model
  - induce charge in pixels (wp)

- **Hitlist per primary**
  - interaction point
  - energy
  - pixel
  - event
  - time

- **Preamp:**
  - charge integration or preamp response
  - SPM and CSM
  - amplitude, ToT and ToA from preamp output

- **Detector:**
  - thresholds
  - counter
  - Medipix/Timepix/Dosepix,...

\[ \sigma = A E_d \left( 1 - \frac{B}{1 + C E_d} \right) \]  \hspace{1cm} (7.1)

The amount of charge that is placed in the initial cloud is determined considering the ionization energy and Fano factor of the sensor material. To increase the simulation speed, the amount of electrons tracked together in a “virtual charge carrier” can be adjusted. A value of 20 electrons for photons has proven itself to be a good compromise between simulation speed and accuracy. The initial distribution sigma of the charge cloud is calculated with:

The model has sufficient accuracy up to a few MeV [Woh+84].
Chapter 7. Geant4 and charge tracking

7.4 Charge carrier tracking and induction

The charge tracking is done using the classic Runge-Kutta-Fehlberg algorithm (RFK45) solving equation 4.8 [Feh70]. The time resolution is constant but can be adjusted via the configuration file. The electric field caused by reverse bias is calculated in every step of the simulation in one-dimension. It can be regarded as parallel throughout the structure. Simulations with COMSOL and TCAD show only a minimal error due to bending of the field lines for the MEDIPiX electrode geometries. A modified version of equation 4.6 is used to calculate the time dependent diffusion and repulsion of the charge carriers when separated:

\[
D'(t) = D + \frac{\mu N q}{24\pi^{3/2}\varepsilon_o \varepsilon_r \sigma(t)}
\]

with the diffusion constant \( D \), the number of charges \( N \) and the time dependent distribution \( \sigma(t) \) [BH09]. After every step the charge is randomly placed in all three dimensions using the \( \sigma(t) \) to generate a Gaussian distribution. If the step exceeds the pixel electrode, its coordinate is set as final at the electrode’s position.

As explained before in section 4.2.3, the induced current at an electrode in a pixel detector depends on a moving charge through its weighting potential. The weighting potential is identical for every pixel with identical geometry. This allows to store the values for one pixel cell in a three dimensional map and reuse them. Unfortunately, there is no analytical solution to obtain these values. Creating the desired pixel geometry in a finite element program and setting the electrode of interest to unity potential while all others are grounded allows to export the electric potential, which then corresponds to the weighting potential of one pixel, into file. We used COMSOL for this purpose and created maps for every combination of pixel size and sensor thickness. Since moving charges can also induce a current in neighbour pixels, the map was chosen to be between 3×3 and 5×5 pixels wide, depending on the geometry, to be able to calculate induction into the neighbours.

The potential map is placed at the pixel coordinate transferred to the WPDigitizer and shifted for every energy deposition. For a virtual charge carrier in motion the potential in every time step is compared to the previous step in all 9 pixels until it arrives at the pixel electrode where it is stopped. For the silicon sensor models recombination and trapping of holes or electrons were
7.5 Preamplifier

In order to build a realistic model of the whole detector a charge sensitive amplifier (CSA) model was be included. The CSA in the detector is realised with a circuit described by Krummenacher [Kru91] that is used for leakage current compensation. The analytical transfer function was kindly provided by the MedPix group at CERN. In the Preamp simulation class the transfer function is convoluted with the induced current output of the Digitizer to obtain the response of the amplifier. The transfer function $h$ can be described with:

$$h(t) = \frac{Q_i}{C_f} \exp\left(w_2 t - \exp\left(w_1 t\right)\right)$$  \hspace{1cm} (7.3)
with an input charge $Q_i$, the feedback capacitance $C_f$. The components $w_1$ and $w_2$ are defined as

$$w_1 = \frac{gC_f}{C_t}$$  \hspace{1cm} (7.4)$$

$$w_2 = \frac{1}{C_f R_f}$$  \hspace{1cm} (7.5)$$

with the transconductance parameter $g$, sensor and parasitic capacitances $C_t$ and feedback capacitance $C_f$ and resistance $R_f$, respectively. The feedback capacitance in the simulation can be adjusted to the same settings as provided in the MEDIPIX gain settings discussed in section 2.2.3. The TIMEPIX detector has a fixed feedback capacitance. The leakage compensation current $I_{Krum}$ used in the Krummenacher circuit influences the feedback resistance which can be approximated with

$$R_f = \frac{I_{Krum}}{20}$$  \hspace{1cm} (7.6)$$

where $I_{Krum}$ corresponds to the electrical current values in the chip not the DAC settings. A predefined amount of noise can be added to the amplifier output signal to precisely model the pixel behaviour. This is done via the ini-file corresponding to the chip specifications. Currently, noise from a Gaussian distribution is added to the CSA output signal. To illustrate the

![Placed charge at different positions](image)

Figure 7.5: Induced current for a charge corresponding to 10 keV placed at different positions inside the pixel volume. In the vicinity of the electrode it can be seen that the faster electrons leave the dense regions of the weighting potential before the holes arrive.
amplifier response no noise has been taken into consideration. Figure 7.6 shows the CSA response to induced currents from energy depositions that were placed at three vertical locations. The computation length convolution with the transfer function of the amplifier can be adjusted. Choosing very short times can cause loss of events while very long pulse times result in long computation times due to the convolution.

The before mentioned $I_{Krum}$ controls not only the dark current compensation in every pixel but also influences the transfer function of the amplifier. It, too, can be adjusted via the configuration file.

In reality the threshold values in the pixels can vary slightly with respect to each other. To simulate this behaviour a mismatch can be set, expressed in the number of elementary charges in the configuration file. An array with the same shape as the pixel matrix is filled with random values of a Gaussian distribution with a sigma corresponding to the requested mismatch.

### 7.5.1 Timepix specific features

The Timepix chips come with two distinctive features, time-over-threshold and time-of-arrival mode. The first mentioned is used in spectral imaging and returns the energy spectrum of the incoming radiation per pixel by measuring the time the CSA output is above a given threshold. TOA returns a time stamp of an arriving energy deposition. In the Timepix1 chips these are two distinct
modes, \textsc{timepix3} on the other hand can do this simultaneously and feeds a constant stream of pixel hits to the computer.

In the simulation TOA and TOT values are calculated simultaneously relative to crossing the threshold. If noise is added to the pulses, the first time the threshold is crossed is used to determine the values.

### 7.5.2 \textit{Medipix specific features}

In the \textsc{medipix3} chips the gain can be changed via programmable feedback capacitors in the amplifier which influences the transfer function. This function is provided in the simulation as well.

Charge summing is another \textsc{medipix3} specific feature which is implemented in the simulation framework [Bal+06]. The output of the charge sensitive amplifier of the four neighbouring pixels is added counted in the pixel with the highest contribution. This means all four pixels contribute with noise with a total noise of $\sqrt{4} = 2$ times the noise of a single pixel. In the simulation we use the sum of the induced currents before convolving it with the transfer function to save computation time.

### 7.6 \textit{Data handling}

To simplify analysis of simulation results, all accessible data can be exported during different simulation steps e.g. CSA pulses and induced currents as well as during the Monte Carlo simulation. Pulses are written to ASCII files while particle data is stored in ROOT histograms or a HDF5 database file. Depending on the configuration a simplified output can be interesting. A file format similar to the Pixelman sparse output settings is available to write pixel, charge, ToT and ToA values to disc [Tur+11].

### 7.7 \textit{Multithreading}

Since version 10.00, the Geant4 framework supports multi-threading which allows for more efficient use of the CPU cores on modern computers and clusters. In figure 7.7 the handling of threads in Geant4 is explained. One control thread controls a number of worker threads that perform the calculations. Geometry, physics and configuration data is hereby shared in a common memory. Random numbers are generated with tunable algorithms and then provided and distributed by the master thread.
7.7. Multithreading

![Diagram of multithreading in Geant4 and Geant4Medipix extension](image)

Figure 7.7: Multithreading in Geant4 and Geant4Medipix extension. Results are merged for direct data export and sent to the charge tracking extension.

<table>
<thead>
<tr>
<th>Table 7.1: Comparison of simulation time for different numbers of threads on an AMD Opteron 6172 cluster with 24 CPUs.</th>
</tr>
</thead>
<tbody>
<tr>
<td>threads</td>
</tr>
<tr>
<td>time (s)</td>
</tr>
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</table>

This principle puts constraints on the data export described in section 7.6. Threads report their data to a singleton class that collects it and writes it to disc. This procedure works well also for larger amounts of threads up to a certain limit as the time they have to wait for access becomes larger. The computation time in seconds for different numbers of threads on a 24-CPU cluster is shown in table 7.1. It can be seen that the computation time linearly decreases until the number of threads equals the number of cores and levels off. However, even with 64 threads on 24 cores computation is still efficient.

Figure 7.8 shows the tracks of 100 photon events inside the detector volume. The volume's size is $10 \times 10$ pixels and the sensor material is defined as cadmium telluride. Tracks deviating from the z-axis are either scattered or fluorescence photons.
Figure 7.8: View through a CdTe detector with interactions of 100 photons of a 80 kVp x-ray spectrum.
VERIFICATION OF SIMULATION

In the previous chapter the functional layout of the Geant4 extension for charge tracking in pixel detectors was discussed.

This chapter discusses the experimental verification of the simulation software with the help of different detector types and geometries, e.g. pixel pitch and size as well as sensor material. The depletion region created by an electric field is measured, simulated and discussed in the first section. Signal formation is discussed and compared with TCAD simulations. With Timepix detectors spectral imaging performance in photon counting and time over threshold mode was compared. The model for the Medipix3RX detector is verified with measurements comparing calibration curves and imaging performance.

8.1 Depletion and electric field

The depletion width in a detector depends on the applied reverse bias, its geometry and doping. As described in chapter 3, the electric field is almost zero in the undepleted part of the sensor. In a pixel detector this can be measured using an inclined or grazing incidence beam. The beam will cross through several pixels and their response depends on if the beam strikes an depleted or undepleted region [Ros+06].

We used detectors with 300 µm high resistive n-type silicon sensors and p-implants at the pixel openings to measure the extent of the electric field in the sensor. The sensor was tilted by 45° and mounted in a beam path shaped by a 10 µm wide slit. Setting it to a an even shallower angle is preferable but was not realized to minimize the distance between slit and sensor and due to mounting restrictions. The X-ray source (Feinfocus Nanofocus) was set to 60 kVp and the spectrum filtered with a 1 mm titanium filter. This was done to minimize the mismatch in count rates in the detector due to higher absorption in pixels at the entrance of the beam compared to those near the exit point.

Additionally, a 5 mm thick lead shield was placed around the slit to absorb scattered photons. The bias voltage of the sensor was stepped up from 0 V to 90 V. The simulation of a slit experiment was set up with the same geometry
Chapter 8. Verification of simulation

Figure 8.1: Experimental set-up to measure the internal electric field of a Medipix detector. The detector can be seen on the left, in the middle the slit and led shield and the X-ray source on the right side.

Figure 8.2: Simulated electric field at full depletion.

and detector configuration. To lower the computational cost the filter and slit was removed and the radiation source configured to send out a line-shaped filtered spectrum instead. The spectrum was simulated with xop 2.3 and confirmed in a measurement with an Amptek X-123CdTe spectrometer.

Figure 8.2 shows the electric field simulated with MEDICI at full depletion. The graph shows the values for a high resistive sensor with an uniform doping of $1.2 \times 10^{11}$ cm$^{-3}$ and a p-doping at the pixel readout side of $1 \times 10^{21}$ cm$^{-3}$ as well as an n+ doping at the cathode of $1 \times 10^{20}$ cm$^{-3}$.
Figure 8.3: Comparison between measured and simulated depletion with an inclined slit. The full depletion in the simulation was set to 15 V.

Figure 8.3a shows the results of the depletion measured with the before mentioned method. It has to be kept in mind that it is only an estimate rather than an exact method. The sensor that was used was 300 µm thick with a 55 µm pixel pitch and showed count rates that indicate full depletion around 10 V to 15 V. In the simulation the electric field is configured using the voltage at full depletion as a parameter. In figure 8.3b it was adjusted to 15 V. The geometry and particle source configuration was as discussed above with about $2.5 \times 10^6$ simulated photons per voltage step. The graph shows that the sensor is fully depleted at a reverse bias of about 15 V.

8.2 Charge induction and amplification

The exact behaviour of the induced current is very hard if not impossible to measure in a pixel detector. Therefore, a MEDICI simulation was used to compare the induced current pulses. One has to keep in mind that MEDICI simulates a 2D slice with a thickness of only 1 µm if not configured with cylindrical coordinates. This corresponds in principle to the design of a strip detector but the weighting potential resembles that of the cross-section through a pixel. A better alternative is to use cylindrical coordinates. The result is a circular electrode with a weighting potential almost identical to a quadratic pixel. Figure 8.4 shows the current in electrons induced in the
electrode of a pixel with charges starting to move from the centre of the device. It can be seen that the curve is slightly different compared to the current in Geant4Medipix (see 7.5). This is due to the method that is used to track the charges in the Monte Carlo extension. The new size of the charge cloud due to diffusion that is calculated in every step is applied to all spatial directions. The electric field strength that affects the movement of carriers is applied to the centre of the charge cloud equally for all charges. In MEDICI on the other hand a mesh is used with charge densities. Different parts of the charge cloud can experience electric field gradients which pull apart the cloud in the field direction and results in a more cone shaped distribution.

The exact shape of the induced current does not have a big impact on the output of the CSA due to its slower timing. Figure 8.5 shows the response of the charge sensitive amplifier to an input current simulated in MEDICI. The simulation results for the pixel located precisely above the impact point of a photon are convoluted with the transfer function of the CSA. It can be seen that the shape of the function is almost identical to the one generated in Geant4Medipix with the difference that the rise is slower in the beginning. However, since the simulation has to be calibrated with a similar procedure as the chip this has no impact on the result.
8.3 Calibration in photon counting mode

In order to use the Medipix chips for spectral imaging it is necessary to calibrate them. This can either be done with the internal test pulses, X-ray fluorescence or other radioactive sources.

We used metal plates with high purity to produce fluorescence photons of different energies as listed in table 8.1. The plates were rotated by 45° and placed about 20 cm from the X-ray source. The detector was mounted 20 cm from the metal forming an angle of 90° with the X-ray source. This arrangement helps to to minimize Compton scattering from the metal and was used for all fluorescence measurements and simulations.

The calibration curve of a Medipix detector is a straight line through the number of counts versus energy. In order to obtain a spectrum in photon counting mode the threshold has to be shifted after recording a number of frames. The result is an integrated spectrum that after differentiation shows the characteristic photopeak.

Table 8.1: XRF metals used for calibration

<table>
<thead>
<tr>
<th></th>
<th>Ti</th>
<th>Fe</th>
<th>Cu</th>
<th>Zr</th>
<th>Ag</th>
<th>Pr</th>
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<tbody>
<tr>
<td>Kα</td>
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</table>

Figure 8.5: CSA output obtained from convolution of induced current in MEDICI and analytical transfer function.
Chapter 8. Verification of simulation

Figure 8.6: Calibration curve for a Medipix3 detector in single pixel mode.

Figure 8.7: Simulated calibration curve for 55 µm and 110 µm pixel sizes.

Figure 8.6 shows the calibration curve for a Medipix3 detector in single pixel mode. The offset can be explained with the non-zero threshold. The chip shows a linear behaviour in photon counting mode over the entire energy range. Figure 8.7 confirms that for simulations with 55 µm and 110 µm pixel pitch the calibration curves in photon counting mode are linear from low to high energies.
8.3.1 Calibration in time over threshold mode

The Timepix detector can record per pixel energy spectra directly when adjusted to ToT mode. The calibration curve of a Timepix detector can be described with the following equation:

\[ f(x) = ax + b - \frac{c}{x - t} \]  \hspace{1cm} (8.1)

with a non-linear behaviour at lower energies and a linear part for higher energies [Jak11]. Figures 8.8 and 8.9 show calibration curves for a Timepix detector. It can be seen that the curve becomes non-linear for low energies transitioning to a linear behaviour at high energies. The simulation does show a slightly different behaviour. This is due to the analytic transfer function explained in equation (7.3) that is used in the convolution with the induced current. Measuring the time over a threshold of the transfer function results in a root function.

8.3.2 Energy resolution

The energy resolution of a detector is an interesting value to compare the performance of different devices. In order to obtain a value the characteristic photo-peak of fluorescence photons is fitted with a Gaussian profile. The
energy of a peak at full width half maximum divided by the mean energy describes the relative energy resolution.

The metals used for in this measurement are listed in table 8.1. Spectra recorded with a Timepix detector in photon counting mode show a slightly better energy resolution than those recorded in time-over-threshold mode which was published by Krapohl et al. [Kra+13]. Table 8.3 shows the calculated resolution of a range of Medipix chips simulated in Geant4Medipix.

### 8.4 Charged particles: electrons and alpha particles

The simulation is very sensitive to the configuration settings for alpha particle interactions. Geant4 uses a value called range cut to determine the energy thresholds for production of secondary particles. Too small values will result in clusters with more energy and cause the image to be distorted from a Gaussian energy distribution that occurs in measurements. The deactivation
of the multiple scattering process with \textit{inactivate} \texttt{msc} causes the energy of a particle to be deposited in its endpoint which again distorts energy deposition. In the \textit{WPDigitizer} the amount of electrons tracked together should be low to get an accurate picture with high energy particles. Additionally, the model used for the initial displacement is increasingly inaccurate at higher energies. Figure 8.10 shows a comparison between measurement and simulation. An Am241 source was used together with a \textit{Timepix} detector to record alpha radiation. The same detector settings were used for both measurement and simulation. The left graph of the figure shows a clipping of a frame with single alpha particle. In the simulation the energy of the alpha particle was set to 5 MeV. In addition to alpha particles the simulation was tested with electrons from a $^{90}$Sr (strontium) source. Both frames in figure 8.11 show the typical shape of energy depositions caused by electrons. Since the source emits a continuous spectrum of electrons with energies up to 0.546 MeV it is not possible to say if the sum of the energies is correct. In the simulation the energy was fixed to the highest possible energy. In figure 8.11b it can be seen that the simulation shows a slightly higher energy deposition per track than the original particle energy.

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Table 8.3: Simulated energy resolution for different detectors and configurations, all simulated. 1) Medipix3, SPM, 110 µm, 2) Medipix3, SPM, 55 µm, 3) Medipix3, CSM, 110 µm, 4) Medipix3, CSM, 55 µm, 5) Timepix1, $I_k=5$ nA, 55 µm, 6) Timepix1, $I_k=0.785$ nA, 55 µm, 7) Timepix3, $I_k=1.2$ nA, 55 µm, 8) Timepix3, $I_k=1.2$ nA, 55 µm

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</tbody>
</table>
Chapter 8. Verification of simulation

Figure 8.10: Comparison between measured and simulated alpha particles. The depletion voltage was 15 V and 20 V respectively. The detector used in the measurement was a Timepix1 in ToT mode at 48 MHz.

Figure 8.11: Comparison between measured and simulated beta-particles emitted by a strontium-90 source. The depletion voltage was 90 V in both. The detector used in the measurement was a Timepix1 in ToT mode at 48 MHz.

8.5 X-ray imaging

As a proof of concept we exposed a gas lighter to the X-ray source. The source was set to 50 kVp and the spectrum used unfiltered. The image in
8.5. X-ray imaging

Figure 8.12 is stitched together from 43 image positions each consisting of 11 exposures that were also flat-field corrected. A flat-field is an image that is taken without object but the same exposure settings. This method allows to correct systematic pixel count variations. The lighter was mounted on a stainless steel post attached to a stepper motor. The slightly darker area on the left hand side of the image is due to a filament change during the experiment and therefore a slight increase of photon flux. The average number of counts in every pixel in the fully exposed part of the detector was about 594,755. The detector was a Medipix3RX with 110 µm pixel pitch set to spectral mode which results in 4 thresholds per pixel. The stitched image shows the lowest threshold which was set to 3.5 keV. The simulation was split into 20 single runs each with $50 \times 10^6$ photons and a detector set-up that measured $512 \times 512$ pixels of 55 µm size. The particle source was configured to be plane shaped with half the detector size to achieve a slight enlargement and the same 50 kVp acceleration voltage used in the measurement. Because of the lower number of photons and total detector size, the resulting image has a lower resolution compared with the measurement.

It is clearly visible that the simulated image contains more noise. In order to get a quantitative measure contrast to noise ratio (CNR) can be used [FNF13]. There are several equations published in different sources, here the following equation is used:

![Figure 8.12: Lighter image taken with Medipix3RX with 110 µm pixel pitch. The image is stitched together from 4×10 single exposures.](image-url)
Chapter 8. Verification of simulation

Figure 8.13: Simulated X-ray image of a lighter. Highlighted regions are noise (1), plastic (2) and metal (3). Simulation done by Armin Schübel.

\[
CNR = \sqrt{\frac{2(S_{im} - S_{bgr})^2}{\sigma_{im}^2 + \sigma_{bgr}^2}} \tag{8.2}
\]

It describes the difference of counts in the object and background divided by the quadratic sum of noise in the image and background. Mainly two regions in the images are interesting to compare since they are very similar in the object and CAD model, one consisting of metal and one consisting of plastic. For the metal region in the cap the CNR is 70.8 in the measurement and 23.0 in the simulation respectively. The plastic region was selected in the gas container of the lighter. Here the values were 16.3 and 2.3. Technically there are no restrictions to image quality. If higher image quality is required in a simulation, it has to be configured to run with more particles.
9.1 Conclusion

The conclusions are divided into two parts, describing the neutron detector simulation and Geant4 pixel detector simulation in separate sections. Finally, suggestions are given to improve the two device simulations and future work is proposed.

9.1.1 Neutron detector

A clean room compatible manufacturing process with a new neutron converter material for semiconductor neutron detection is presented in this thesis. The layer structure and effectiveness of the device was simulated with Geant4. A prototype of the detector was manufactured in Mid Sweden University’s clean-room and analysed in the laboratory with IV measurements and neutrons. Further testing has been done at the Czech Metrology institute in Prague in a neutron field. The results show that it is possible to evaporate TiB$_2$ on silicon devices as a neutron converter material. The measurements showed a very good agreement between simulation and fabricated device.

9.1.2 Pixel detector simulation

In the second part of this thesis a simulation framework method for spectral imaging hybrid pixel detectors is presented. The Geant4 code extension for charge tracking was developed from the idea to combine Monte Carlo simulation with TCAD charge transport. To avoid converting data between different types of simulation programs and simulation speed issues, charge tracking was implemented as an add-on to Geant4. Geant4Medipix is able to simulate particle passage through matter as well as charge transport and readout electronics response. The code extension is able to simulate charge transport of X-ray photons with very good results. Results obtained with high energy and heavy charged particles deviate from measurements with increasing energy.
Chapter 9. Conclusion and Outlook

9.2 Future work

In order to increase the sensitivity of the neutron detector different improvements can considered. Backside illumination is the simplest way of achieving better effectiveness without changing its design. The thickness of the converter can be increased to convert more neutrons with the disadvantage of smearing out the alpha peak and losing energy resolution. A more effective way of increasing alpha conversion is to change the planar design into a three-dimensionally structured geometry. Pyramid structures can be achieved with anisotropic etching techniques and are relatively simple to come by. These can be filled or lined with the converter material. Even better effectiveness is expected of deep trenches in the semiconductor that can be filled with a neutron converter.

The Geant4Medipix simulation framework showed good results for X-ray simulations with TIMEPIX and MEDIPIX chips combined with silicon sensors. However, charged particle simulation becomes increasingly imprecise and time consuming for increasing energies. In future versions the model used for alpha particles and heavy charged particles needs adjustments since it tends to overestimate the size of the initial charge cloud. Another bottleneck is the simulation speed for high energy depositions. A solution could be to modify the charge tracking algorithm to be able to run parallel diffusion tracks. Only very basic models for high-Z materials are implemented at this point. These have to be verified and extended. Since trapping of charges is observed in some of these materials, modelling of this behaviour might be of importance. A measure to speed up the simulation could be to introduce a method using a so-called charge induction map. Hereby, a map of the pixel volume is calculated that stores information of the induced current of a charge originating from a certain coordinate. The disadvantage is, without modification, there is no information about the timing characteristic of the induced current.

Ultimately, the goal is to combine thermal neutron simulation with the Geant4Medipix framework to design high resolution neutron imaging sensors.
### 9.3 Authors' contribution to included publications

Authors' contribution to the research papers included in this thesis are listed in table 9.1.

#### Table 9.1: Authors contributions to included papers.

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Chapter 9. Conclusion and Outlook

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| VIII | AS                              | Implementation, simulations and measurements |
|      | DK                             | Idea, implementation, simulation, measurements and supervision |
|      | EF                             | Implementation, simulations and discussion |
|      | CF                             | Supervision and discussions |
|      | GT                             | Supervision and discussions |

| IX   | DK                             | Simulations and measurements |
|      | AS                             | Simulations and measurements |
|      | EF                             | Simulations and measurements |
|      | CF                             | Supervision and discussion   |
|      | GT                             | Supervision and discussion   |

ADDITIONAL PUBLICATIONS

The following is a list of publications by the author that are not included in this thesis.


Additional publications


PATENTS

The following is a list of publications by the author that are not included in this thesis.

ACRONYMS

CCD
Charged Coupled Device

CdTe
Cadmium-Telluride

CSA
Charge sensitive amplifier

CSM
Charge summing mode

CZT
Cadmium-Zinc-Telluride

ESS
European Spallation Source

GaAs
Gallium-Arsenide

Geant4
GEometry ANd Tracking

LET
Linear energy transfer

MPX
Medipix

SPM
Single pixle mode

TCAD
Technical Computer Aided Design
Acronyms

$\text{TiB}_2$
Titaniumdiboride

TOA
Time-of-Arrival

TOT
Time-over-threshold

TPX
Timepix

XRF
X-ray fluorescence
BIBLIOGRAPHY


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