

Modelling of the signal induced by the charged particles in silicon detector by Gaussian clouds dynamics method



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Oświadczenie

Ja, niżej podpisany, **mgr Przemysław Kulig**, doktorant Wydziału Fizyki, Astronomii i Informatyki Stosowanej Uniwersytetu Jagiellońskiego, oświadczam, że przedłożona przeze mnie rozprawa doktorska pt. **„Modelling of the signal induced by the charged particles in silicon detector by Gaussian clouds dynamics method”** jest oryginalna i przedstawia wyniki badań wykonanych przeze mnie osobiście, pod kierunkiem dr hab. Tomasz Kozika (oraz wcześniej dr hab. Zbigniewa Sosina). Pracę napisałem samodzielnie.

Oświadczam, że moja rozprawa doktorska została opracowana zgodnie z Ustawą o prawie autorskim i prawach pokrewnych z dnia 4 lutego 1994 r. (Dziennik Ustaw 1994 nr 24 poz. 83 wraz z późniejszymi zmianami).

Jestem świadom, że niezgodność niniejszego oświadczenia z prawdą, ujawniona w dowolnym czasie, niezależnie od skutków prawnych wynikających z ww. ustawy, może spowodować unieważnienie stopnia nabytego na podstawie tej rozprawy.

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(podpis doktoranta)

Abstract

The numerical implementation and extension of the Gaussian Clouds Dynamics (GCD) model [1] of current pulse generation in silicon detectors is presented aiming at theoretical understanding of Pulse Shape Analysis (PSA) techniques. The approach is based on Ramo-Shockley theorem and takes into account Coulomb interaction between electron and hole clouds in the electric field of a silicon detector. Several factors influencing the collection process of carriers induced by charged particles are investigated for possible improvements of the isotopic separation capability. The Plasma Delay Effect (PDE) was found to govern the identification by their impact on the time dependence of the signal. Opportunities for model developments are proposed.

Streszczenie

Metoda Analizy Kształtu Impulsu (PSA), stosowana do identyfikacji fragmentów reakcji jądrowych, może być teoretycznie opisana i zrozumiana przy pomocy modelu Dynamiki Chmur Gaussowskich (GCD) [1]. Podejście to opiera się na twierdzeniu Ramo-Shockley'a i uwzględnia oddziaływanie kulombowskie pomiędzy chmurami elektronów i dziur w polu elektrycznym detektora krzemowego. Przy pomocy numerycznej implementacji tego modelu zbadano kilka czynników wpływających na proces zbierania nośników ładunków wygenerowanych przez rejestrowane cząstki. Wyniki tych badań mogą być wykorzystane w celu ulepszenia izotopowej zdolności rozdzielczej. Stwierdzono, że Efekty Opóźnienia Plazmy (PDE) mają decydujący wpływ na parametry czasowe otrzymywanego sygnału. Zaproponowano także możliwe kierunki dalszego rozwoju modelu GCD.

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Chapter 1

Introduction

Silicon detectors have played a crucial role in the field of charged particle detection, contributing significantly to advancements in theoretical physics and practical applications across various sciences. These devices utilise sophisticated techniques derived from fundamental physical principles, which have evolved together with progress in core science, computational methods, and electronics design.

This thesis focuses on the microscopic modelling of current pulses induced by heavy ions in semiconductor detectors, with a special focus on silicon. It explores the Gaussian Clouds Dynamics (GCD) model [1], which integrates the Ramo-Shockley theorem with the dynamics of electron and hole clouds in the electric fields of the detectors.

Understanding these interactions is crucial for advancing Pulse Shape Analysis (PSA) techniques - essential methods for the accurate identification of charged particles, which have been under significant developments in recent decades, alongside the classical ΔE - E method. By investigating factors such as the Plasma Delay Effect (PDE), which significantly influence particle identification through PSA, this research aims to refine the theoretical frameworks used in particle detection. The goal is to provide directions for potential enhancements in particle identification, recommendations for device design, and verification of the GCD model outcomes, while also outlining prospects for its further development.

This thesis is organised as follows:

In Chapter 2, the fundamental processes governing the interaction of charged particles with matter are discussed, including the historical background and details of the Bethe-Bloch formula.

Methods of particle identification in silicon detectors are examined in Chapter 3. The classical ΔE - E technique and Pulse Shape Analysis approach are described in detail, with a focus on key factors influencing the results,

such as channelled/random configuration and front/rear side experimental setups.

Chapter 4 provides an overview of the models utilised throughout this study, covering both the theoretical foundations and their software implementation.

The experimental environment used for model comparison and the initial simulation runs to reproduce the identification matrices are introduced in Chapter 5.

The impact of carrier mobility on system evolution and identification capability is explored in Chapter 6, correlating with diffusion coefficients. The free GCD model parameter (variance mobility) is tested for several potential values, and the influence of mirror reflections is also analysed.

Chapter 7 describes the process of signal reconstruction using the Ramo-Schockley theorem and the preamplifier response function.

The impact of temperature on carrier mobility, utilising the Arora model, is investigated in Chapter 8.

Finally, the conclusions and some proposals for further model developments are given in Chapter 9.

Chapter 2

Interactions of charged particles with the matter

Heavy charged particles primarily interact with matter through Coulomb forces with the negative charges of electrons in the atoms they encounter. While it is possible for these particles to engage with atomic nuclei, such as in Rutherford scattering or reactions triggered by alpha particles, these events are relatively rare and generally do not significantly influence the performance of detectors. Instead, the functionality of charged particle detectors mainly depends on interactions with electrons. As a charged particle penetrates a medium, it engages multiple electrons simultaneously. During each event, the electron is subjected to a force due to the particle's positive charge as it moves nearby. The intensity of this force can either elevate the electron to a higher energy level within the atom (a process known as excitation) or eject the electron from the atom entirely (ionization). The energy imported to the electron reduces the kinetic energy of the charged particle, thereby slowing it down. The greatest amount of energy that can be transferred to an electron from a charged particle in a single collision is approximately $1/500$ of the particle's energy per nucleon, which is a small fraction of the particle's total kinetic energy. Consequently, the charged particle must experience numerous such interactions to significantly deplete its energy while moving through the absorber. Continuously interacting with multiple electrons, the particle progressively loses velocity until it is completely stopped. Charged particles are characterised by a specific range in a given absorber material. The range, which will be more precisely discussed in the next paragraphs, represents the distance beyond which no particles will penetrate.

In 1904, W. H. Bragg made a pioneering investigation into the interaction of ionizing radiation with matter, focusing on the behaviour of alpha

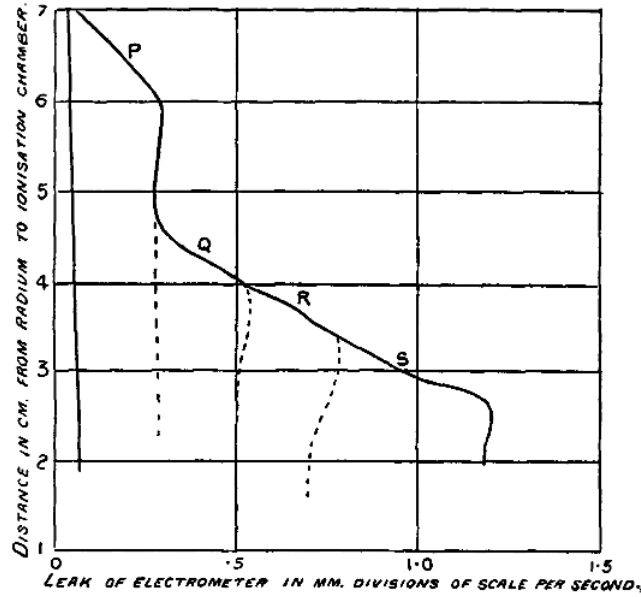


Figure 2.1: One of the ionization curves presented by Bragg in [2].

particles emitted from radium [2]. Bragg developed an experimental method to measure the ionization of air by these particles at varying distances from their source. His findings revealed that alpha particles travel through matter in a straight path, maintaining their ionizing potential until they expend all their energy. This research was instrumental in the development of what is now known as Bragg's curve, which graphically represents the energy loss of ionizing particles as they pass through matter, demonstrating the pattern of energy loss until the particles are completely stopped. Figure 2.1 displays the historical depiction of Bragg's curve, while subsequent 2.2 illustrate the more contemporary methods of visualization commonly used in current publications. The Bragg curve is particularly known for the 'Bragg peak', a distinct feature that shows a sharp increase in ionization near the end of the path of the particle, just before it stops. This peak occurs because as the particle slows down, its interaction cross-section with the electrons in the material increases, leading to a higher probability of energy transfer and thus a greater rate of energy loss per unit path length.

The theoretical estimate of the energy that a heavy charged particle loses when passing through a medium is based on the application of the Born approximation to describe collisions of this particle with electrons in atoms. The Born approximation simplifies the description of particle collisions by assuming that the scattered particle's wave function, both before and after the collision, can be approximated as plane waves. This is practical in scenarios

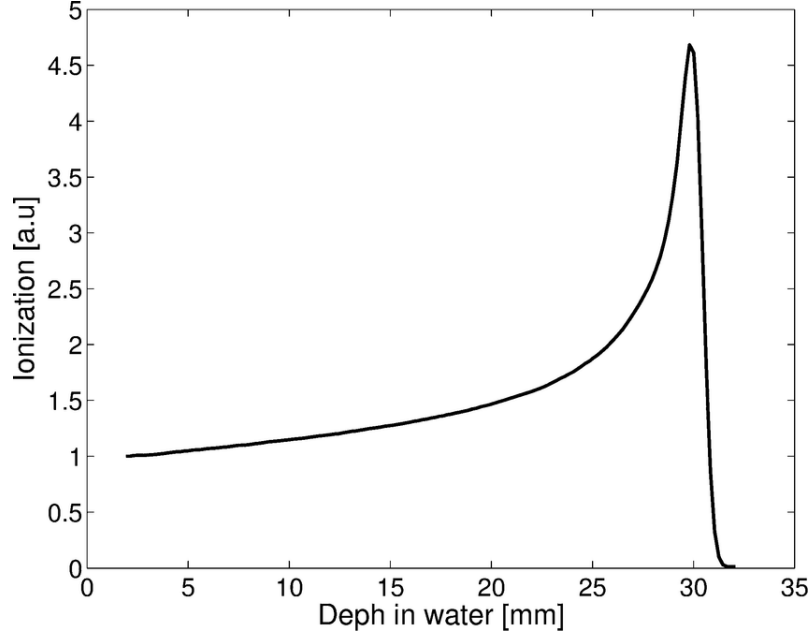


Figure 2.2: Bragg peak of 62-MeV proton beam acquired in a water-tank with the ionization chamber in Catania facility [4].

where the particle's interaction with the scattering potential, such as that from electrons in atoms, is relatively weak, allowing for more straightforward calculations of the energy loss and that approach was applied by Bethe in his original research [3]. The atom involved in the collision was described in its initial state by the unperturbed wave function for the ground state, and in the final state by the wave function for one of the excited states. Then, in order to determine the average energy loss per unit length of the particle's path, the author multiplied the cross-section for a given energy loss by the value of this transferred energy and summed the results obtained for all possible types of interactions. The application of the Born approximation implies that the amplitude of the scattered wave, describing the heavy particle, must be small in comparison to the amplitude of the incoming wave, meaning that the energy loss introduces only a minor disturbance.

The other conditions for the Born approximation applicability are: high velocity of the particle (incident particle kinetic energy is much larger than the potential energy variations due to the scattering centres), small charge (a smaller charge on the scattering particle reduces the strength of its interaction with the scattering centre) and charge constancy during collisions (electrostatic potential involved in the interactions does not change). Calculations become simpler if the velocity of the heavy charged particle is large

compared to the velocity of electrons in the atom. The basic conditions are as follows:

$$\frac{ze^2}{\hbar v} \ll 1 \quad (2.1)$$

where: z - particle charge, e - electron charge, v - velocity of particle and

$$E \gg \frac{M}{m_e} E_i \quad (2.2)$$

where: E - particle energy, M - particle mass, m_e - rest electron mass, E_i - ionization potential of the electron. The application of these conditions led Bethe to demonstrate that at non-relativistic speeds, the mean energy loss per unit length of the particle's path (to ensure consistency, the notation and expression used here follow those found in [5]) can be expressed as:

$$-\frac{dE}{dx} = \frac{4\pi e^4 z^2 \rho N_A Z_{abs}}{m_e v^2 A_{abs}} \ln\left(\frac{2m_e v^2}{I}\right) \quad (2.3)$$

where: e - electron charge, z - particle charge, ρ - material density, N_A - Avogadro number, Z_{abs} - material atomic number, v - velocity of particle, I - excitation potential, A_{abs} - material atomic mass. The considerations performed for the relativistic case led to the following formula:

$$-\frac{dE}{dx} = \frac{4\pi e^4 z^2 \rho N_A Z_{abs}}{m_e c^2 \beta^2 A_{abs}} \left[\ln\left(\frac{2m_e c^2 \beta^2}{I}\right) - \ln(1 - \beta^2) - \beta^2 \right] \quad (2.4)$$

where $\beta = \frac{v}{c}$.

The unit of $\frac{dE}{dx}$ (which is also called the stopping power) is $[\frac{MeVcm^2}{g}]$ and it can be described as an energy per meter, modified by a factor $\frac{1}{\rho}$.

It is essential to consider two important corrections when applying the Bethe-Bloch formula - shell and density effects.

Starting with the shell one, it becomes relevant at lower energies, challenging the assumption that atomic electrons are free. This effect grows significant when the velocity of the incoming particle matches the orbital speeds of the electrons within the atoms. As a result, there is an increase in energy loss, particularly noticeable as the particle's energy approaches the ionization potentials of the electrons in the material. The shell correction modifies the logarithmic term in the Bethe-Bloch formula to reflect the binding energies of the electrons, which influence the interaction cross-section between the particle and the atomic electrons. This correction typically reduces the calculated energy loss and is crucial at lower particle velocities.

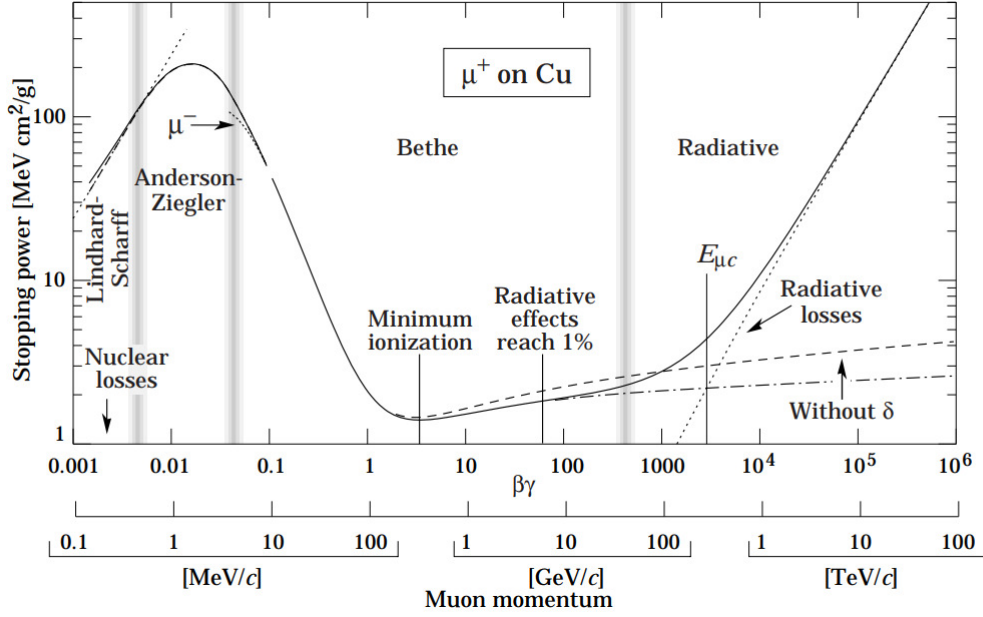


Figure 2.3: Illustration of the corrections to the Bethe-Bloch formula due to shell and density effects: the energy loss rate of muons in copper. The solid line represents the total energy loss, while the dashed lines indicate individual effects contributions [6].

Secondly, the density effect correction, often represented as $\delta(\beta)$, addresses the polarization of the medium induced by a fast moving charged particle. As the particle's velocity reaches relativistic speeds, the electrons in the medium cannot adjust instantaneously to the changing electric field. This lag leads to a lower actual energy loss than predicted by the original Bethe-Bloch formula, which assumes an instantaneous static response from the medium.

These two effects are well illustrated on commonly cited graphics presented here in Figure 2.3 [6], where the stopping power of the muon passing through copper media is shown.

Chapter 3

Charged particles identification

3.1 $\Delta E - E$ identification technique

ΔE - E technique for charged particle identification is well established since Bragg curve was described in 1904 [2] and still remains a frequently used method in experimental projects. This approach considers two detectors, when particles are punching through the first one and are stopped in the second detector. The energy partition between these two detectors is an identification factor as stopping power differs. This method utilises the principle that a material's stopping power varies with the nature of the incident particle and relies on Bethe formula introduced in Eqs. (2.3) and (2.4).

Figure 3.1 [7] illustrates the energy loss profiles of carbon and neon ions, both entering at the same incident energy, within a specific material. The fundamental principle of the ΔE - E method involves segmenting the material into two layers and recording the energy loss in each layer. This arrangement of detector material layers is known as a telescope. The distribution of energy across the two detectors then varies depending on the type of particle detected.

Figure 3.2 displays the correlation between the energy loss in the first layer and the total incident energy, which enables the discrimination between Neon and Carbon. In this representation, known as the ΔE - E matrix, different particles form quasi-parabolic lines that are characteristic of their charge Z and mass A .

We continue using the notation from [5] and reformat Eq. (2.3) by introducing two constants:

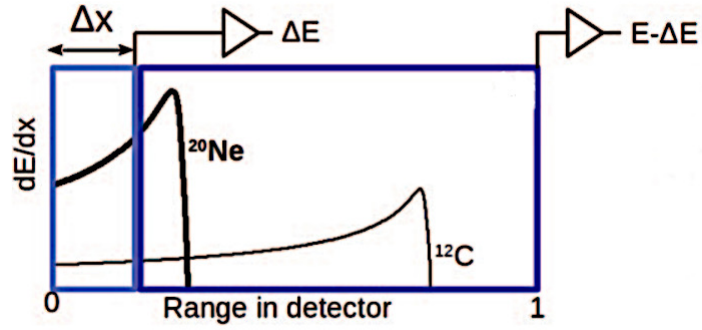


Figure 3.1: Visualisation of the mass detector system presenting the ΔE -E matrix configuration [7].

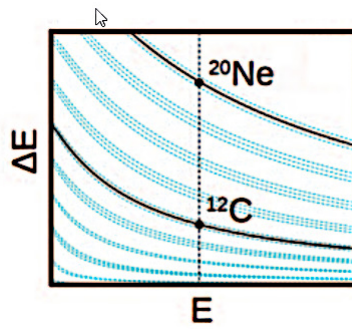


Figure 3.2: Illustrative example of mass discrimination in the ΔE -E matrix. Quasi-parabolic lines are marked for the case of Neon and Carbon [7].

$$B = \frac{2\pi\rho e^4 N_A Z_{abs}}{m_e A_{abs}} \quad (3.1)$$

$$C = \frac{4m_e}{I} \quad (3.2)$$

leading to the following form of Eq. (2.3):

$$-\frac{dE}{dx} = \frac{2Bz^2}{v^2} \ln\left(\frac{Cv^2}{2}\right) \quad (3.3)$$

and after applying formula for kinetic energy:

$$-\frac{dE}{dx} = B \frac{Mz^2}{E} \ln\left(\frac{CE}{M}\right) \quad (3.4)$$

Identification function for $\Delta E - E$ is derived using this form of the Eq. (3.4):

$$BMz^2 = -\frac{dE}{dx}(E) \frac{1}{\ln\left(\frac{CE}{M}\right)} \quad (3.5)$$

We introduce T denoting the thickness of the detector and ΔE representing the average energy loss. Calculating the integral of Eq. (3.5) from $x = 0$ to $x = T$ leads to:

$$BTMz^2 = B \int_0^T Mz^2 dx \quad (3.6)$$

$$BTMz^2 = - \int_{E_T - \Delta E}^{E_T} E \frac{1}{\ln\left(\frac{CE}{M}\right)} dE \quad (3.7)$$

Eq. (3.7) can be calculated numerically, or one can notice $\frac{CE}{M} \gg 1$, therefore $\ln\left(\frac{CE}{M}\right)$ can be expanded into series. These considerations lead to following result:

$$TMz^2 \sim (E_T + k\Delta E)\Delta E \quad (3.8)$$

More detailed discussions on the form and modifications of functions used for charge and mass identification in the ΔE -E method may be found e.g. in [8, 9].

It is relevant to consider the influence of channelling effects in the detector configuration.

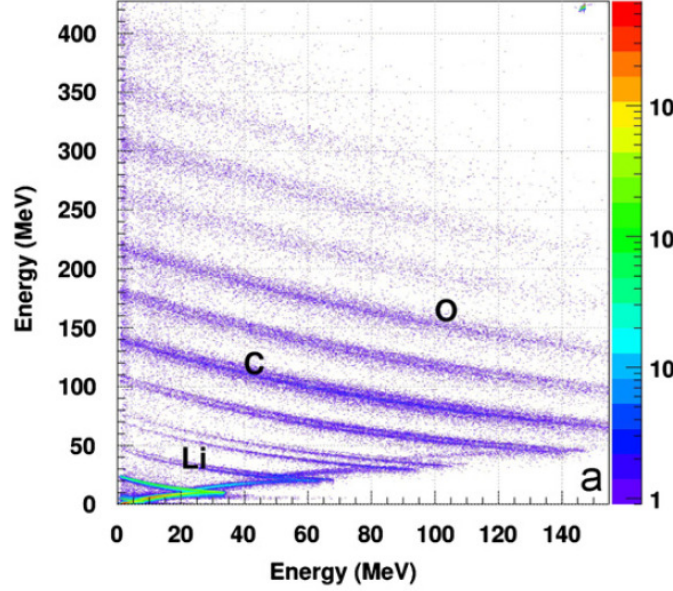


Figure 3.3: Standard $\Delta E - E$ plots obtained in silicon detector ($300 \mu m \Delta E$, $500 \mu m E$) with channelled configuration [10].

When ions travel through a detector parallel to its crystal planes or axes (channelled configuration), they experience a unique set of interactions. Due to these specific trajectories, there is an increase in fluctuations in measured parameters such as energy loss. This can negatively impact the performance of the identification method like the ΔE - E one. In contrast, when ions enter the detector in a random configuration (their paths do not align with any specific crystal axes or planes) the fluctuations in energy and signal rise-time are minimized. This configuration is beneficial for achieving clearer and more consistent detection outcomes.

Those effects can be well observed e.g. in [10] where the detectors have been installed on a custom-designed mechanical system enabling control over the orientation. With this mechanical setup, and given the known crystal orientation of the detectors relative to the support frame, it was possible to adjust the tilt of the detectors to switch between 'channelled' or 'random' configurations as required.

Illustration of the difference in the identification performance is presented in Figure 3.3 and 3.4 [10].

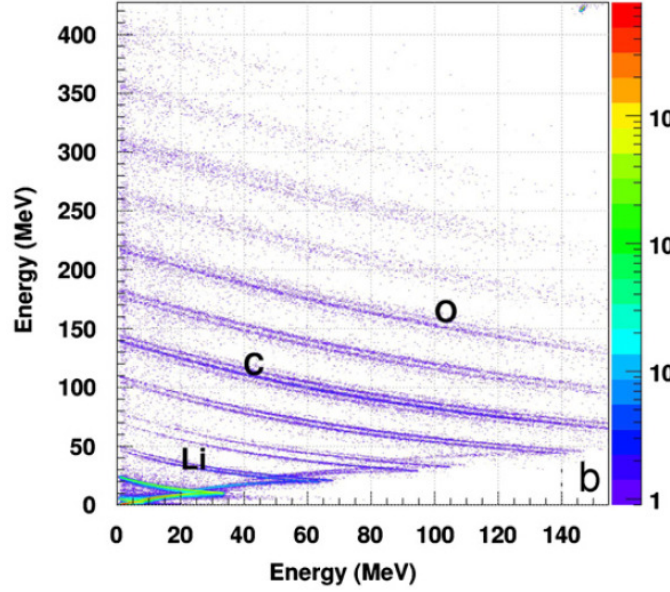


Figure 3.4: Standard $\Delta E - E$ plots obtained in silicon detector ($300 \mu m \Delta E$, $500 \mu m E$) with random configuration [10].

3.2 Pulse Shape Analysis

Pulse Shape Analysis (PSA) technique was proposed in 1963 in [11]. The method is based on the fact that when an ionizing particle enters a semiconductor radiation detector, it generates a voltage pulse. The height of this pulse is determined by the particle energy, while its shape is influenced by the particle range within the detector. Therefore, the characteristics of the voltage pulse carry valuable information about the type of particle, allowing for its identification based on energy and trajectory.

To present it in more detail, we can say that an impinging particle generates electrons and holes within the semiconductor material. The external field then separates these free charges, consequently generating a voltage signal on the electrodes. The time it takes for this signal to rise, known as the rise time, is influenced by the time required to collect the charge. This collection time is dependent on the distance the charge carriers need to travel. The final pulse height is directly proportional to the energy lost by the particle within the detector. Thus, the voltage pulse provides information about both the particle's energy and its range. Given that these two characteristics define the nature of a particle, the type of particle can be determined through

an analysis of the pulse.

Authors derived the energy loss per unit length $\frac{dE}{dx}$ from the empirical range-energy formula $R = aE^b$ (a, b - constants):

$$\frac{dE}{dx} = -\frac{1}{a^{1/b}b(R-x)^{(b-1)/b}} \quad (3.9)$$

A few years later [12] it was shown that Eq. (3.9) leads to relation showing the induced charge $Q(t)$, associated with the movement of electrons and holes in the detector:

$$Q(t) = \frac{qE}{E_0}[E_n(t) + H_n(t)] \quad (3.10)$$

where E_0 - energy required to create an ion pair.

$E(t)$ and $H(t)$ describe the normalized components of the voltage signal at time t , originating respectively from electrons and holes, whereby:

$$E_n(t) + H_n(t) \rightarrow 1 \quad (3.11)$$

$$t \rightarrow \infty$$

Considerable advancements were published in [13] and [14], which provided a comprehensive explanation of the physics underlying the rise time process of the charge signal. Additionally, it was suggested that the minimum energy threshold for charge identification is achieved when the particle strikes the detector surface from the side where the electric field is weakest, known as the reverse configuration. This aspect will be further discussed in the next section.

In general those considerations paid attention to the importance of collection time (or pulse rise time) of carriers which generally in semiconductor detectors is a function of several influencing factors:

$$\tau = f(\tau_E, \tau_P, \tau_{RC}, \tau_A) \quad (3.12)$$

where τ_E - carriers collection time in the detector field, τ_P - plasma dissociation time related to the ionization density across particle trajectory, τ_{RC} - time related to the capacitance of the detector sensitive layer and to the resistance of the detector, τ_A - characteristic time of external amplifier and cabling connections.

Charged particles enter silicon detector and create a plasma column (visualisation presented in Figure 3.5 [15]), with ionization density depending on energy, charge and mass of a particle, described by the Bragg curve which plots the energy loss of the particle during its travel through matter. The current pulse rise time depends on mutual interactions of induced carriers and is referred to the Plasma Delay Effect (PDE). The stopping power is important in both methods, ΔE -E and PSA. However, the latter is more sensitive to the ionization density distribution enhancing the influence of PDE on the pulse formation.

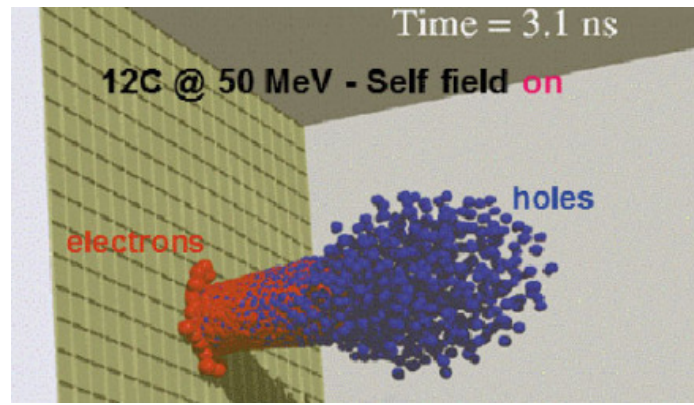


Figure 3.5: 3D simulated plasma column for 50 MeV 12C in silicon detector [15].

In silicon detectors PDE effect can be observed as a pulse rise time slow-down for increasing Z as a consequence of the increased density of formed plasma. The pulse formation is also influenced by other factors like location of the ionization track in the detector, purity and doping homogeneity of the silicon material as well as the response of the preamplifier to the input current pulse. The PSA method is being developed at present as it is more economic (only one electronic channel) and offers lower energy threshold (no ΔE layer) comparing to ΔE -E technique.

It is worth noting that the crystal orientation can also affect the shape of the signal, creating an important factor in the PSA technique (as mentioned in the section 3.2 regarding the ΔE -E case).

Typical experimental identification correlations with well-pronounced back-bending are presented in Figures 3.6 and 3.7 [16]. It is clearly evident how random configuration can improve the identification resolution.

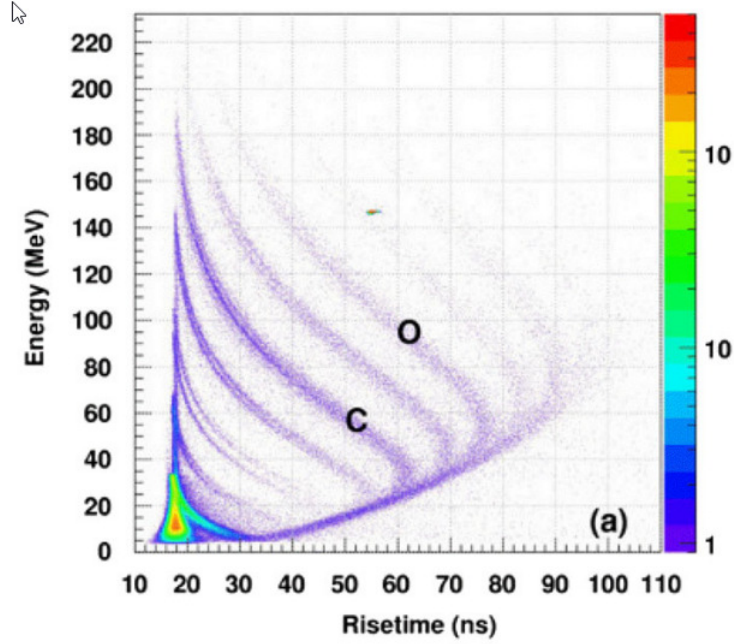


Figure 3.6: Pulse shape analysis identification diagram (energy vs. charge rise-time). Detector ($500 \mu m$) in channelled configuration [16].

3.3 Front and rear side configuration

Strong arguments for using the 'reverse mode/rear mount' configuration in detectors (i.e. hit from the lower energy field side), schematically presented in Figure 3.3, were proposed in [13].

Extensive research in this area conducted over the last decades has led to reliable and comprehensive conclusions regarding particles identification using ΔE - E and PSA techniques. These results, utilising both front and rear side impinging configurations, have been presented e.g. in [17] - different responses were observed when particles entered the detector through the front side, distinguished by a high electric field, compared to the rear side, characterised by a low electric field. Notably, while previous studies have independently explored both configurations using separate devices, the cited investigation uniquely employed the same detector and electronics to conduct their research.

First observation regarding $\Delta E - E$ technique are presented in Figures 3.9, 3.10, where one can see the similar identification plots in both configurations. As a result, the same quality of the energy measurement was obtained.

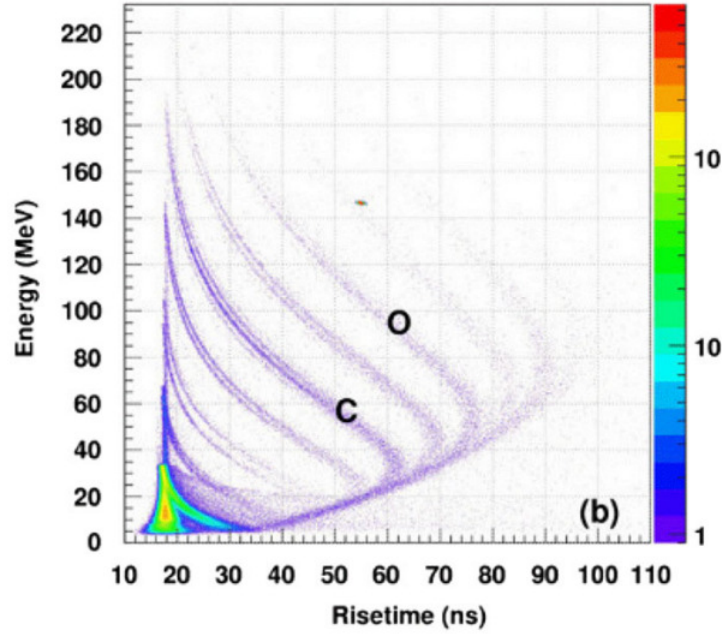


Figure 3.7: Pulse shape analysis identification diagram (energy vs. charge rise-time). Detector ($500\ \mu\text{m}$) in random configuration [16].

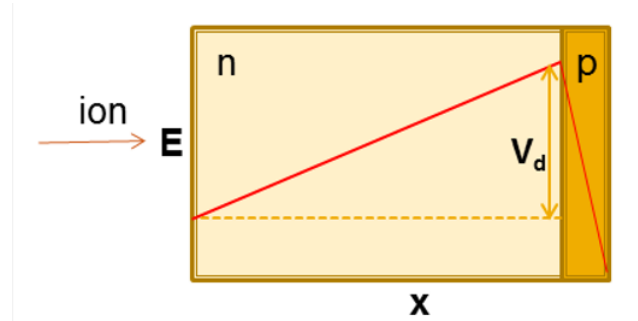


Figure 3.8: Schematic illustration of the reverse mode configuration in detectors.

The zoomed plot at low energy for light nuclei, shown in Figures 3.11, 3.12, confirms the same level of resolution.

Continuation of this research using the PSA method leads to completely different conclusions. A very large increase of the measured rise time (200 ns versus 100 ns) for the rear side injection configuration was observed. That is presented in Figures 3.13, 3.14. Furthermore, the relationship between

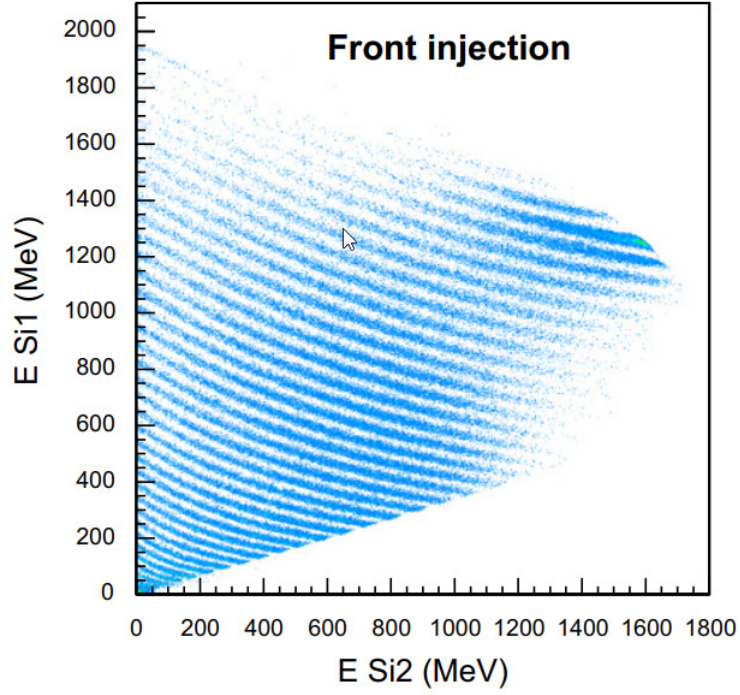


Figure 3.9: $\Delta E - E$ identification matrix in front mount configuration [17].

energy and charge rise time varies significantly between the two cases. In the front side injection, the charge rise time continues to decrease with decreasing particle energy. On the contrary, for rear side injection, starting from high kinetic energies, we observe a rise-and-fall trend of the rise time which, for slow ions, produces a ridge where all values merge together, whatever the particle is. In both cases a 'no identification' zone is visible for each line at low energy, defining a Z dependent identification threshold.

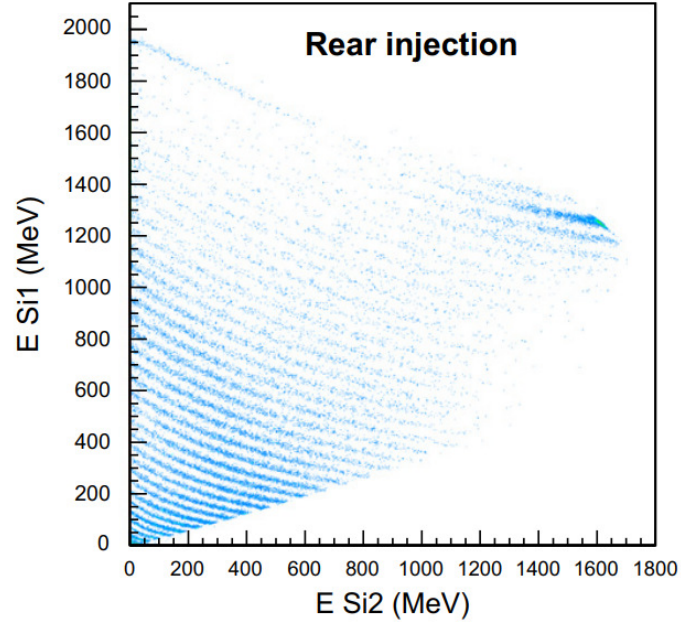


Figure 3.10: $\Delta E - E$ identification matrix in rear mount configuration [17].

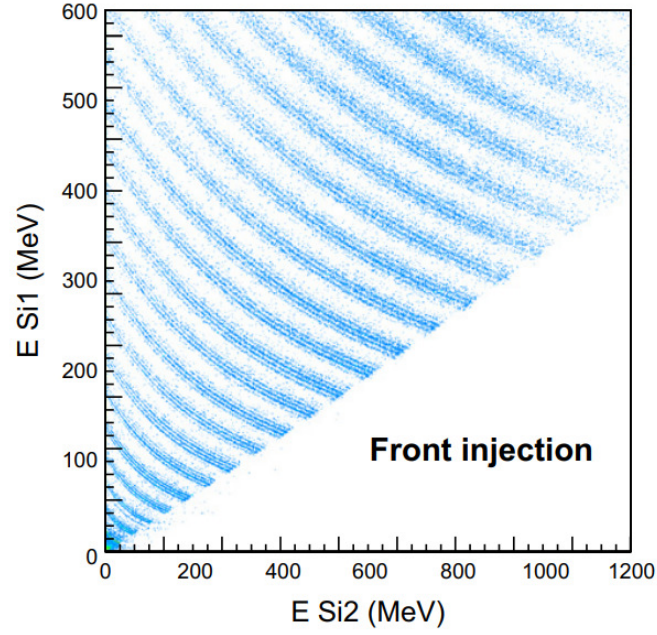


Figure 3.11: Zoomed plot of Figure 3.9

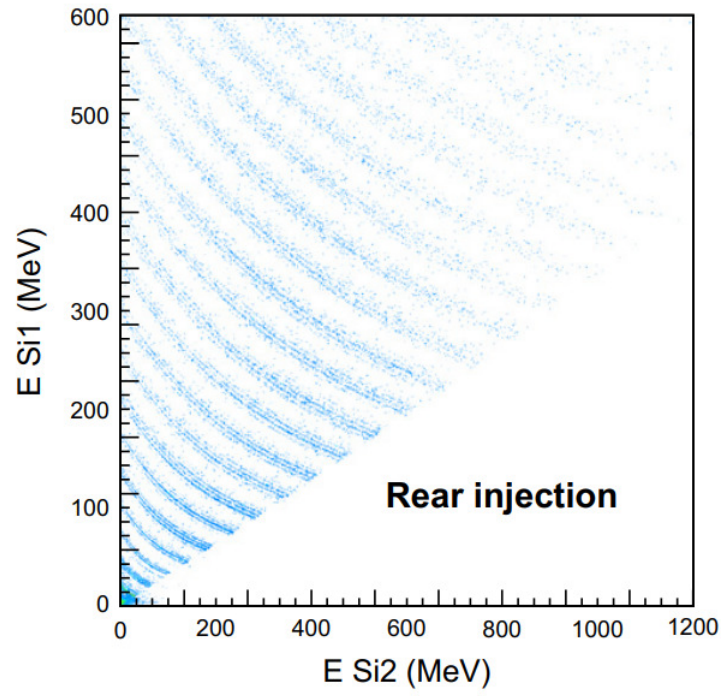


Figure 3.12: Zoomed plot of Figure 3.10

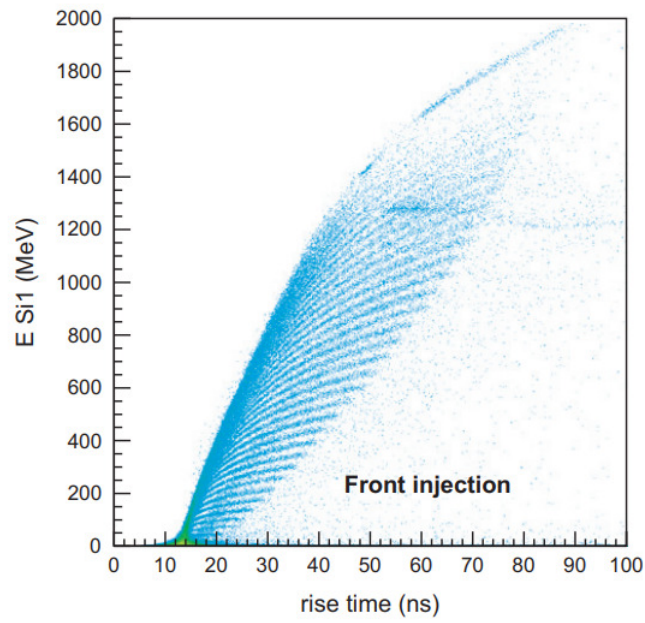


Figure 3.13: Front configuration of the PSA [17].

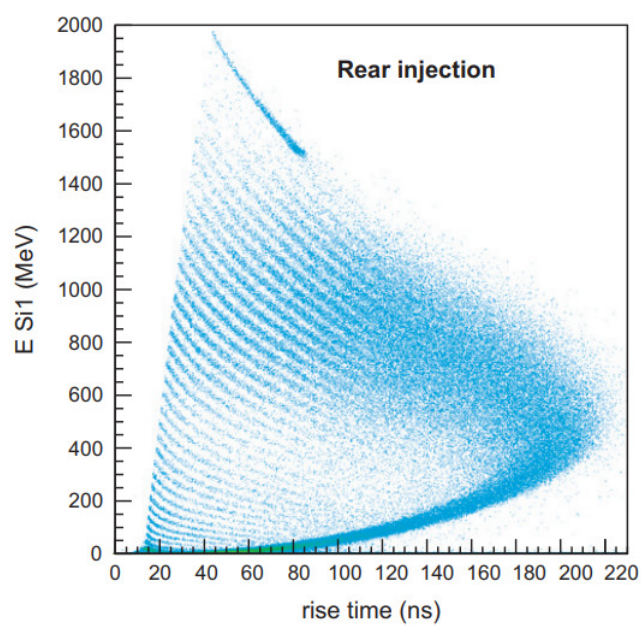


Figure 3.14: Rear configuration of the PSA [17].

Chapter 4

Gaussian Clouds Dynamics model overview

4.1 Rationale for model development

In recent decades, there were a few attempts to describe and model the Plasma Delay Effect, which affects time characteristics of the charge carriers collection. These investigations are essential to improve applicability of PSA methods. The polarization of the electron-hole pair column induced by heavy ions in a silicon detector was considered in [18, 19] and connected to the relative dielectric permittivity. The dissociation of pairs was supposed to take place with a constant probability in a time unit. The coordinate dependence of the modified electric field was found as the solution of the one-dimensional Maxwell's equation for the electric field in this inhomogeneous medium. The PDE originates in this approach from the local electric field decreasing. The GCD model is more like the one presented in [15]. Both models introduce 'clusters' and consider interactions among these charge clouds to calculate clusters motion.

4.2 Evolution description

According to the model proposed in [1] we take into account not only diffusion but also drift in the electric field in the perpendicular direction to the column axis. This approach is not limited to a finite number of clusters - it describes the evolution of the continuous distribution of charge densities ρ_e , ρ_h for

electrons and holes, respectively, using a superposition of Gauss functions G_e and G_h . Ionization is assumed to be proportional to the energy loss

$$B(x) = \frac{1}{w} \frac{dE}{dx}(x) \quad (4.1)$$

where w - average energy for an electron-hole pair production in silicon ($w = 3.62$ eV); $\frac{dE}{dx}(x)$ - energy loss at given position [20]. Initial charge densities (after stopping of the ion) are written:

$$\rho_e(\mathbf{r}, t=0) = -\rho_h(\mathbf{r}, t=0) = - \int B(x') \delta(x-x') \delta(y) \delta(z) dx' \quad (4.2)$$

where $\mathbf{r} = [x, y, z]$. As the analogy to Eq. (4.2), the evolution of carrier densities may be presented by using the superposition of Gauss functions G_e and G_h :

$$\rho_e(\mathbf{r}, t) = \int B_e(x', t) G_e(x-x', y, z, t) dx' \quad (4.3)$$

$$\rho_h(\mathbf{r}, t) = \int B_h(x', t) G_h(x-x', y, z, t) dx' \quad (4.4)$$

where ionization

$$-B_e(x, t=0) = B_h(x, t=0) = B(x) = \frac{1}{w} \frac{dE}{dx}(x) \quad (4.5)$$

is proportional to the energy loss at a given position.

Gaussians G_e and G_h are described in the following way:

$$G_e(x-x', y, z, t) = \frac{1}{\sqrt{(2\pi)^3 \sigma_e^3(x, t)}} \exp \left(-\frac{(x-x')^2 + y^2 + z^2}{2\sigma_e^2(x, t)} \right) \quad (4.6)$$

$$G_h(x-x', y, z, t) = \frac{1}{\sqrt{(2\pi)^3 \sigma_h^3(x, t)}} \exp \left(-\frac{(x-x')^2 + y^2 + z^2}{2\sigma_h^2(x, t)} \right) \quad (4.7)$$

For $\sigma_e \rightarrow 0$ and $\sigma_h \rightarrow 0$ (and $t \rightarrow 0$) G_e and G_h are considered as representations of δ function:

$$G_e(x-x', y, z, t=0) = G_h(x-x', y, z, t=0) = \delta(x-x') \delta(y) \delta(z) dx \quad (4.8)$$

The following assumptions are made: propagation of electrons and holes generated in detector is represented by Gaussian clouds motions; centroids and variances are calculated separately for both carriers; the time evolution of Gaussian centroids is ruled by drift; the time evolution of Gaussian variances is ruled by both diffusion and drift.

4.3 Characterization of electric fields

In order to calculate the Gaussian drift velocity it is necessary to introduce the effective electric field description. We consider the rear-mounting configuration, meaning that incident ions enter the detector from the low electric field side. It was proved that such configuration gives better results in PSA method [17, 21]. In that case static field can be described:

$$E_{static}(x) = \frac{2V_dx}{d_{Si}^2} + \frac{V - V_d}{d_{Si}} \quad (4.9)$$

$$V_d = \frac{q_0 N_D d^2}{2\varepsilon_r \varepsilon_0} \quad (4.10)$$

where d_{Si} - detector thickness, V - the bias voltage and V_d - the depletion voltage and $V > V_d$ (in our calculations $d_{Si}=310$ μm , $V = 190\text{V}$, $V_d=128\text{V}$), N_D - concentration of donors, ε - permittivity, q_0 - electron charge. Plasma influences the electric field and the goal is to describe its evolution. The model uses an interaction potential of the clouds similar to the quantum molecular dynamics approach [22]:

$$\begin{aligned} v(r_{01}, r_{02}, \sigma_1, \sigma_2) &= \frac{e^2 \mathbb{Z}_1 \mathbb{Z}_2}{(2\pi\sigma_1\sigma_2)^3} \iint \frac{\exp\left(\frac{-(\mathbf{r}_1 - \mathbf{r}_{01})^2}{2\sigma_1^2}\right) \exp\left(\frac{-(\mathbf{r}_2 - \mathbf{r}_{02})^2}{2\sigma_2^2}\right)}{|\mathbf{r}_1 - \mathbf{r}_2|} d^3\mathbf{r}_1 d^3\mathbf{r}_2 = \\ &= e^2 \mathbb{Z}_1 \mathbb{Z}_2 \frac{\text{erf}\left(\frac{r_{12}}{\sqrt{2}\sigma}\right)}{r_{12}} \end{aligned} \quad (4.11)$$

where $\mathbb{Z}_1, \mathbb{Z}_2$ denote the electron and hole cloud charges with Gaussian distributions centred at a relative distance $r_{12} = |\mathbf{r}_{01} - \mathbf{r}_{02}|$ and characterized by variances σ_1^2, σ_2^2 and $\sigma = \sqrt{\sigma_1^2 + \sigma_2^2}$. Therefore, the generalized interactions of continuous Gaussian charge distributions are implemented instead of interactions between a finite number of point charges. The following form will express effective electric field E_x acting on the Gaussian located at a point a :

$$E_x(a, c, d, p, q, \sigma_a, \sigma_i) = -\frac{1}{Z_a} \frac{\partial V_C}{\partial a} = -\frac{e^2}{\varepsilon} \int_c^d dx (px + q) \frac{\partial}{\partial a} \frac{\text{erf}\left(\frac{|x-a|}{\sqrt{2}\sigma_s}\right)}{|x-a|} \quad (4.12)$$

Since $\frac{\partial}{\partial a} = -\frac{\partial}{\partial x}$, the above formula can be expressed as:

$$E_x(a, c, d, p, q, \sigma_a, \sigma_i) = \frac{e^2}{\varepsilon} q \left(\frac{\text{erf}\left(\frac{|d-a|}{\sqrt{2}\sigma_s}\right)}{|d-a|} - \frac{\text{erf}\left(\frac{|c-a|}{\sqrt{2}\sigma_s}\right)}{|c-a|} \right) + \frac{e^2}{\varepsilon} p \int_c^d dx x \frac{\partial}{\partial x} \frac{\text{erf}\left(\frac{|x-a|}{\sqrt{2}\sigma_s}\right)}{|x-a|} \quad (4.13)$$

Which gives:

$$E_x = \frac{e^2}{\varepsilon} q \left(\frac{\operatorname{erf}\left(\frac{|d-a|}{\sqrt{2}\sigma_s}\right)}{|d-a|} - \frac{\operatorname{erf}\left(\frac{|c-a|}{\sqrt{2}\sigma_s}\right)}{|c-a|} \right) + \frac{e^2}{\varepsilon} p \left(d \frac{\operatorname{erf}\left(\frac{|d-a|}{\sqrt{2}\sigma_s}\right)}{|d-a|} - c \frac{\operatorname{erf}\left(\frac{|c-a|}{\sqrt{2}\sigma_s}\right)}{|c-a|} \right) +$$

$$- \frac{e^2}{\varepsilon} p \int_c^d dx \frac{\operatorname{erf}\left(\frac{|x-a|}{\sqrt{2}\sigma_s}\right)}{|x-a|} \quad (4.14)$$

The total effective electric field modified due to the presence of plasma can be obtained by summing up contributions of charges located in all intervals (c_i, d_i) and of their mirror reflections induced in the detector. At this juncture, it is particularly relevant to emphasize that the current model approximation is specifically designed to take into account only the nearest mirror reflections. This limitation is noteworthy and will be revisited in details later in this manuscript to explore potential implications and future enhancements to the model. This is illustrated in Figure 4.1: considering the detector of thickness d , with electrodes at 0 and d will lead to the generation of the mirror charges at $-x$ and $-x + 2d$ (with reverse charge and with the same variance).

Information on the effective field propagation allows us to write the expression for average velocity of Gaussian representing electrons at point x_i :

$$v_{xei} = \mu_{xe} E_{xei} \quad (4.15)$$

where E_{xei} - effective electric field for electrons in the x direction; μ_{xe} - electrons mobility. Formula for holes can be written by the analogy:

$$v_{xhi} = \mu_{xh} E_{xhi} \quad (4.16)$$

where E_{xhi} - effective electric field for holes in the x direction; μ_{xh} - holes mobility. By accurately determining the drift velocity, it becomes possible to calculate the evolution of the charge deposited across each interval Δx_i .

4.4 Perpendicular direction in charges motion

It is now important to calculate how diffusion and transport processes in an electric field affect the spread of charge distributions with their centroids at each Δx_i . The velocity $v_{\sigma ei}$ (describing expansion in the perpendicular direction) comprises three distinct components:

$$v_{\sigma ei} = v_{\sigma ei}^E + v_{\sigma ei}^D + v_{\sigma ei}^T \quad (4.17)$$

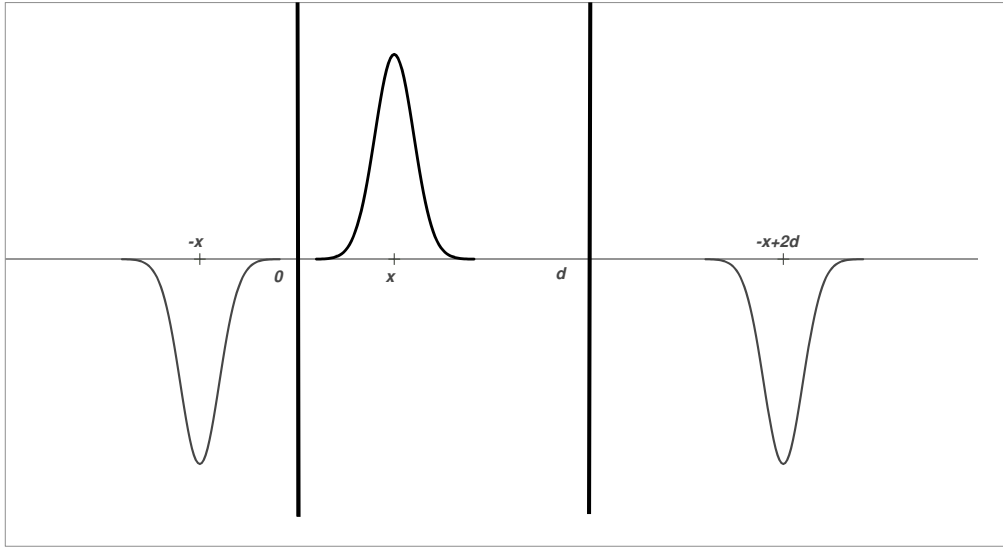


Figure 4.1: Visualization of model assumption: according to model [1] particle impinging the detector induces charges which are considered to be Gaussian clouds. The model assumption takes into account only interactions between the nearest reflections. The opportunities to apply further reflections to the model are discussed later in this dissertation.

The first component, $v_{\sigma ei}^E$ represents the factor related to effective electric field considered in 4.14 and is directly proportional to the electric field $E_{\sigma ei}$ acting on the charge:

$$v_{\sigma ei}^E = \mu_{\sigma e} E_{\sigma ei} \quad (4.18)$$

The second part, $v_{\sigma ei}^D$, is derived from solving Fick's second law of diffusion, which governs the behaviour of Gaussian density distributions:

$$v_{\sigma ei}^D = \frac{D_e}{\sigma_{ei}} \quad (4.19)$$

where D_e denotes electron diffusion coefficient.

The third item, $v_{\sigma ei}^T$, is responsible for description carriers transport.

Analogous formulas are used to determine the propagation dynamics for holes.

4.5 Model implementation

The program is specifically engineered to deploy the Gaussian Clouds Dynamics (GCD) model, which investigates the interactions between charged particles and the internal structures of silicon detectors. This model focuses on how charge carriers - electrons and holes - move and diffuse under the influence of an electric field, capturing the key dynamics of evolution.

It starts by reading input parameters from the user (text file), which include environmental conditions, detector specifications, and initial particle states. These parameters are crucial for accurately setting up the simulation environment. However, it is worth mentioning that there are many numerical values hardcoded within the application, which is an area for future enhancements. The core of the program calculates the evolution of charge distributions using differential equations leading to computing system evolution (carriers propagation). The output of the implementation is structured as an ntuple, which is a type of data structure particularly favoured in particle physics for its efficiency in storing and accessing multi-variable datasets. Each ntuple consists of a tuple of values where each entry corresponds to a specific variable or measurement from the simulation.

Single simulation execution takes typically more than 4 hours. Most of the calculations presented in this dissertation were performed using ZFGM (Department of Hot Matter Physics) computational cluster (shiva.if.uj.edu.pl) and IN2P3 Computing Centre cluster.

The following steps can be researched and implemented to make the simulation more valuable for modelling purposes:

- Software migration and modernization. During the development and enhancement phases of our project, we conducted an analysis regarding porting our existing Fortran codebase to C++. This analysis focused on several key aspects such as performance benchmarks, development time, compatibility with existing systems, and the availability of modern programming features that could enhance maintainability and scalability. Although the decision was to retain Fortran, this task could be considered a valuable subject for a Master's or Bachelor's thesis in Computer Science, offering students a great opportunity to engage with real-world software engineering challenges in scientific computing.

- Integrated visualization tools. Introducing output visualization directly into the simulation software could add significant value. Providing immediate visual feedback can help users better understand their data and refine their hypotheses in real time. This idea could be combined with a 'dry-runs' approach (low density of calculation points) to quickly see the trends of evolution in a particular setup.

- Performance optimization. In-depth static and dynamic analysis could be executed to tune the overall performance. Exploring parallel computing could improve the efficiency of the differential equation-solving processes, aiming to significantly reduce simulation time. The Open MultiProcessing (OpenMP) [23] framework is one possible solution that supports multi-platform shared-memory parallel programming in C/C++, and Fortran and has become commonly used for adding parallelism to existing Fortran software.

- Numerical calculations stability improvement. In several simulation trials, it has been observed that the output generated by the application may be impacted by numerical instabilities. Further research in this domain is needed to identify the underlying causes and develop effective solutions. Initial analysis should focus on investigating memory allocation for large arrays and errors associated with numerical precision. A preliminary measure to enhance computational stability would involve assessing the impact of converting from 64-bit double precision (real*8) to 128-bit quadruple precision (real(kind=16)). This change should be evaluated not only for its potential to increase accuracy but also to ensure it does not adversely affect performance metrics.

- Automation and workflow management. The computational demands of running extensive simulations (e.g., those needed to produce an energy-collection time matrix) can also be substantial. Each simulation run with varying parameters consumes significant time and computational resources.

To streamline this process, automating the execution and management of simulation runs becomes essential.

In summary, these proposed enhancements aim to improve the software's functionality, efficiency, and user engagement. By focusing on modernization, visualization, performance optimization, and automation, the program is poised to more effectively meet the evolving demands of scientific computing. This development will not only advance the capabilities of the simulation but also enrich the user experience and outcome accuracy.

Chapter 5

Application of the GCD model

5.1 Experimental data

The results of model calculations may be qualitatively compared with experimental data obtained in [10]. Pulse shape identification plots (energy vs. rise-time) presented in Figure 4.1 were obtained with the Si detector characterized by similar parameters as assumed in the model calculations. The achieved exceptional identification capabilities is the result of several procedures which were developed during the preparatory phase of the investigation [24]. One of most important is random cutting of silicon wafers inclined with respect to the main crystalline axes. This treatment makes the crystal behaves as an amorphous material from the point of view of the registered particle and reduces the effects associated with crystal orientation [25]. We have used silicon detectors with very good dopant homogeneity obtained with the n-TD process, detectors selected with non-destructive laser-based mapping of the resistivity as a function of the position on the silicon, all it allowed to achieve inhomogeneities as small as 1% [26]. All detectors were reverse mounted, so the particles enter from the low-field side. In this way it is possible to maximize the rise-time differences of the charge signals produced by different stopped nuclei of the same energy [11, 27, 13, 28, 29, 21, 18, 15]. Applied aluminum layer of about 30 nm on both sides of the detectors reduced sheet resistance allowing to preserve good timing properties. It appeared also that permanent control of the constancy of the electric field inside the detectors as a function of time was necessary. It is because any change of the detector reverse current, which usually increases with time, induces a change in the voltage drop across the bias resistor (20 M Ω) and this drop must be continuously compensated. The specially designed preamplifiers, with charge and current output, were located inside the vacuum chamber

as close as possible to the detector in order to minimize the impact of the length of the connecting cables on the shape of the signals, on the noise and on the pick-up of disturbances. The entirely digital treatment of the sampled pulse shapes turned out to be a key issue because numerical treatment of the signals allowed for optimal extraction of timing and energy information. We use the charge collection time as a coordinate presenting the results of calculations, rather than the experimentally measured risetime, noting that these two observables are strongly correlated. The correlation between the collection time and the rise time is quantitatively obtained by calculating the preamplifier response to the time-dependent signal from the detector. The preamplifier transmission function may be obtained taking into account the realistic electronic parameters of front-end electronics [19].

5.2 GCD simulations

Z. Sosin proposed in [1] a new method of signal simulation based on Ramo-Shockley theorem where, in addition to the external electric field (induced by the static voltage applied to the detector electrodes) forming the active volume of the detector, the Coulomb interaction between electron and hole clouds have also been taken into account. The results presented in that dissertation refer to calculations carried out for the case of an overdepleted detector. Model calculations conducted for Boron and Carbon isotopes are presented in Figures 5.1 and 5.2. However, here we would like to show the simulations presenting collection times separated for electron and holes.

On Figures 5.3 and 5.4, one can observe that collection times are much shorter for electrons, data calculated for two Carbon isotopes: ^{10}C and ^{12}C , which means holes collection times will considerably dominate the simulated propagation.

In general, carrier mobility depends on the field strength, doping and other material parameters. In this research thesis we do not analyse these dependencies for the sake of clarity and we use values typical for silicon detectors taking carriers mobilities as fixed values. We rather focus on the model predictions concerning most important factors determining charge and isotope resolution of the PSA method.

The following aspects related to the dynamics of plasma column are investigated: plasma erosion related to the different collection rates of electrons and holes and interaction of charge carriers with mirror reflections generated on the detector electrodes. All along this thesis, the calculations concern reverse mounting configuration of silicon detectors, so that the particles enter from the low-field side. In this way it is possible to maximize the rise time

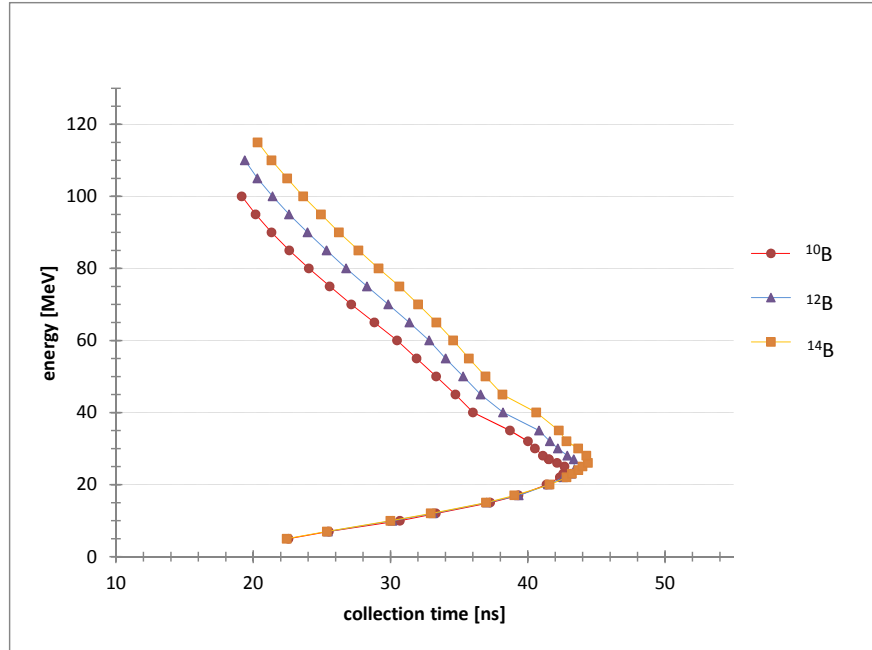


Figure 5.1: Model calculation for Boron isotopes ^{10}B , ^{12}B , ^{14}B - energy versus collection time identification matrix (silicon detector: thickness 310 μm , $V = 190\text{V}$).

differences of the charge signals produced by different stopped nuclei of the same energy [17, 27, 13, 28, 29, 21].

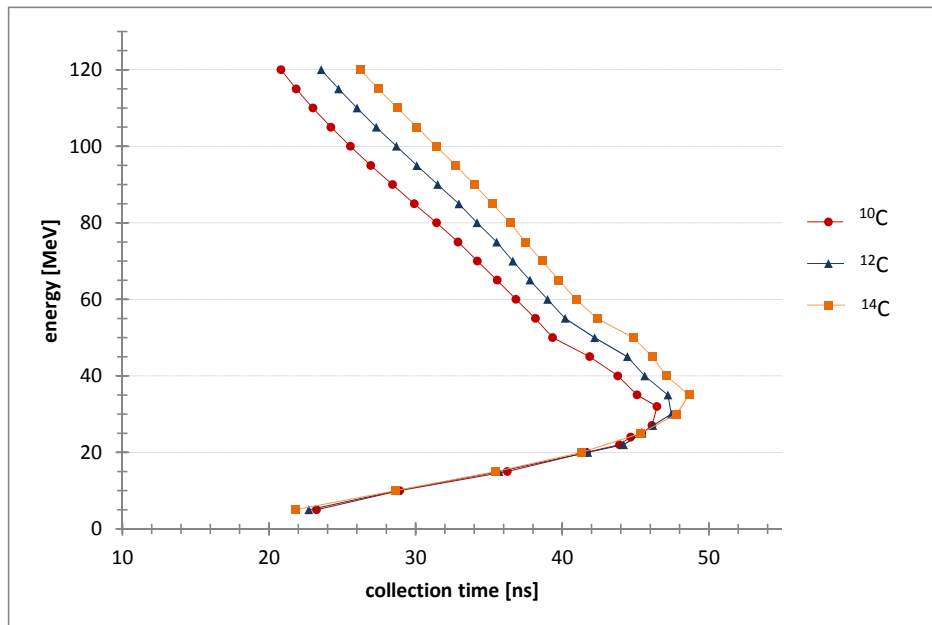


Figure 5.2: Model calculation for Carbon isotopes ^{10}C , ^{12}C , ^{14}C - energy versus collection time identification matrix (silicon detector: thickness 310 μm , $V = 190\text{V}$).

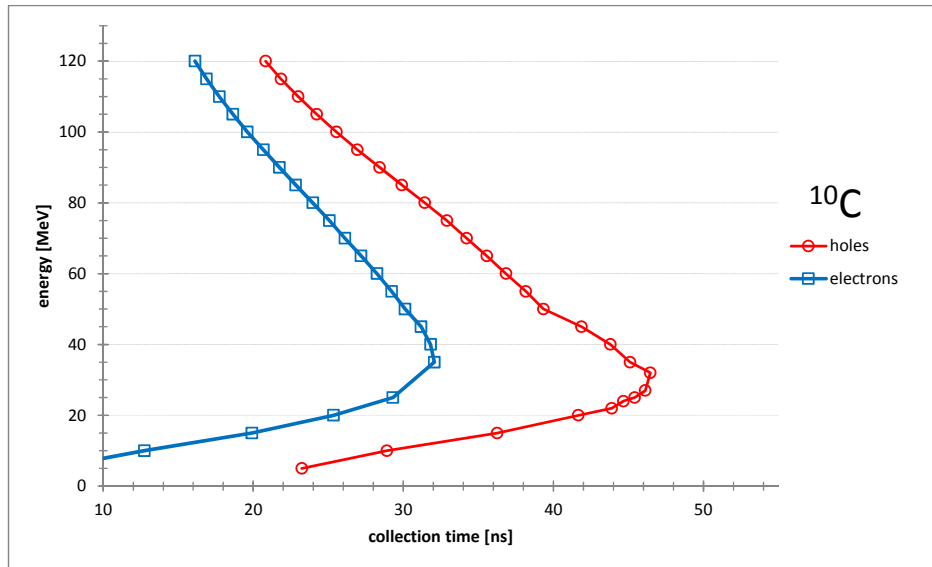


Figure 5.3: Model calculation for ^{10}C - energy versus collection times separated for electron and holes (silicon detector: thickness 310 μm , $V = 190\text{V}$).

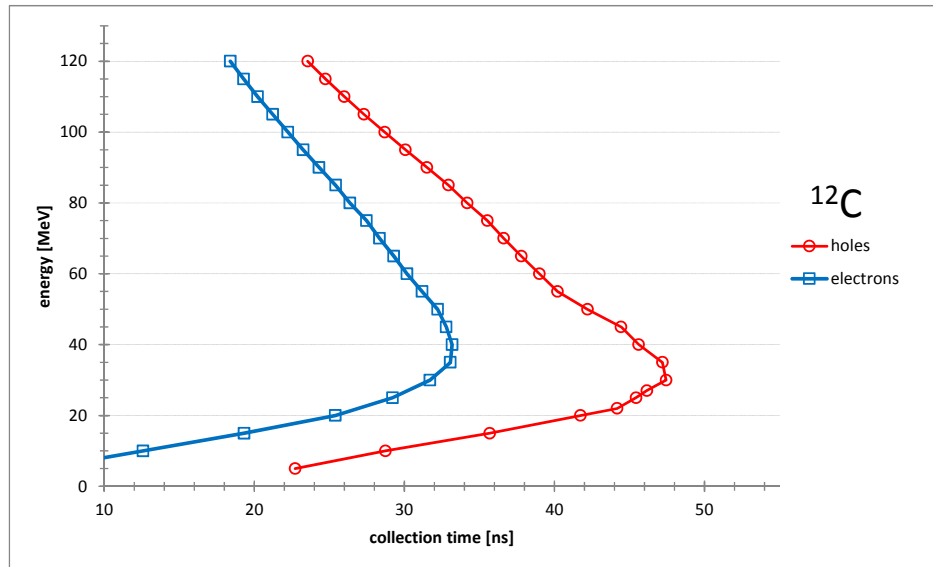


Figure 5.4: Model calculation for ^{12}C - energy versus collection times separated for electron and holes (silicon detector: thickness 310 μm , $V = 190\text{V}$).

Chapter 6

Optimization of PSA performance.

6.1 Base calculations

In order to conduct the actual calculations some physical parameters have been set. Table 6.1 presents their values and includes material constants (μ_{xe} , μ_{xh} , D_e , D_h) and the model parameters ($\mu_{\sigma e}$ and correlated $\mu_{\sigma h}$). Further discussion shows how the modifications of some of these factors can impact the system evolution. Table 6.2 provides the assumptions on the detector parameters, which were used in the simulations. Identification matrices (i.e. energy versus carriers collection time) were already presented in Figures 5.1 and 5.2 for Boron (^{10}B , ^{12}B , ^{14}B) and Carbon (^{10}C , ^{12}C , ^{14}C) isotopes.

Table 6.1: Base parameters of the GCD model

Parameter	Value
Electrons mobility	$\mu_{xe} = 135 \left[\frac{\mu m^2}{V ns} \right]$
Holes mobility	$\mu_{xh} = 47.5 \left[\frac{\mu m^2}{V ns} \right]$
Diffusion coefficient for electrons	$D_e = 3.49 \left[\frac{\mu m^2}{ns} \right]$
Diffusion coefficient for holes	$D_h = 1.228 \left[\frac{\mu m^2}{ns} \right]$
Electrons variance mobility	$\mu_{\sigma e} = 2 \left[\frac{\mu m^2}{V ns} \right]$
Holes variance mobility	$\mu_{\sigma h} = \mu_{\sigma e} \frac{\mu_{xh}}{\mu_{xe}}$

Table 6.2: Detector properties applied in the model calculations

Parameter	Value
Thickness	310 μm
Depletion bias	128 V
Operating bias	190 V
Resistivity	2.5 k Ω cm

6.2 Charge carriers mobilities

In the next step the model is applied to investigate the charge carriers evolution for different values of electrons and holes mobility. So far all calculations were performed with the base parameters from Table 6.1. However, the fixed value of mobility represents a significant approximation. In general, the electron and holes mobilities depend on the donor and acceptor concentrations, impurity concentrations, defect concentration and electron and hole concentrations. They also depend on the temperature and electric field, and usually they are determined empirically. Therefore, it is important to verify how changing electron and holes mobilities can impact the evolution. Figure 6.1 presents results for doubled and halved mobilities with respect to the standard values for Silicon. As expected, one can notice that smaller values result in longer collection times and back-bending point appears at smaller energies. Consequently, preparation of the detector material with the lowest possible carriers mobility may give some improvement of identification capabilities. It has already been observed in [30, 31] that the collection time, obtained by means of rear side injection undepletion, leads to better performance of the PSA.

This effect is further illustrated in Figure 6.2, where the correlation between collection times and mobilities is presented.

Figure 6.3 presents the results for different values of diffusion coefficients D_e and D_h . It may be observed that smaller values of the diffusion coefficient cause a shift of the back-bending point towards lower energies. On the basis of the above observations, one can conclude that any enhancement of the Plasma Delay Effect causes lowering of the identification energy threshold. The PDE is influenced by the bias voltage of the detector and, from low values, is limited according to assumed depletion depth. At higher bias voltages, the limitation comes from drift velocity saturation caused by phonon emission [32]. The linear relationship between the average carrier velocity and the applied field breaks down when high fields are applied. As the electric field is increased, both the average carrier velocity and energy rise. When the

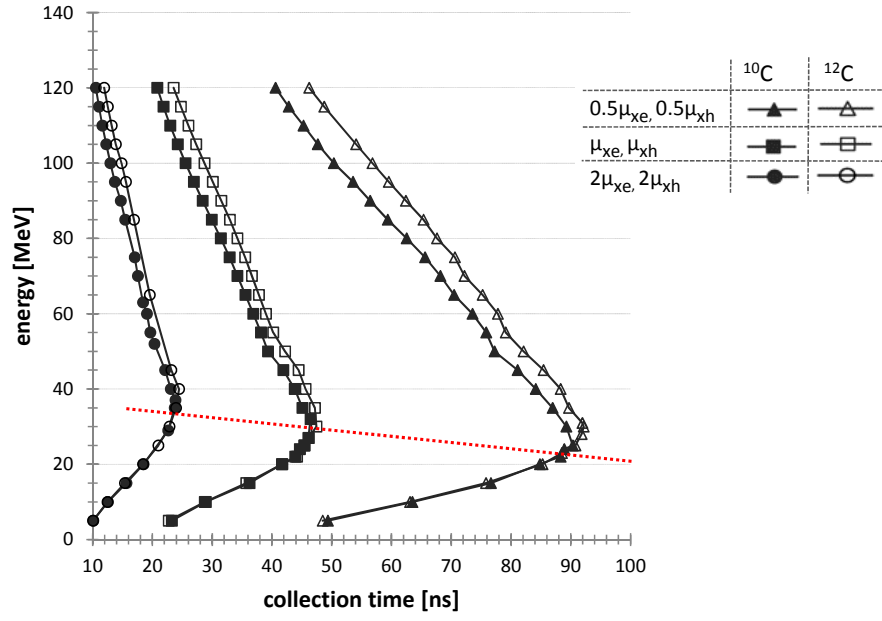


Figure 6.1: PSA identification plot for different values of electron and hole mobility. Smaller values result in longer collection times and back-bending point appears at smaller energies. Base parameters are: $\mu_{xe} = 135 \left[\frac{\mu\text{m}^2}{\text{Vns}} \right]$; $\mu_{xh} = 47.5 \left[\frac{\mu\text{m}^2}{\text{Vns}} \right]$ (detector properties as in 6.2).

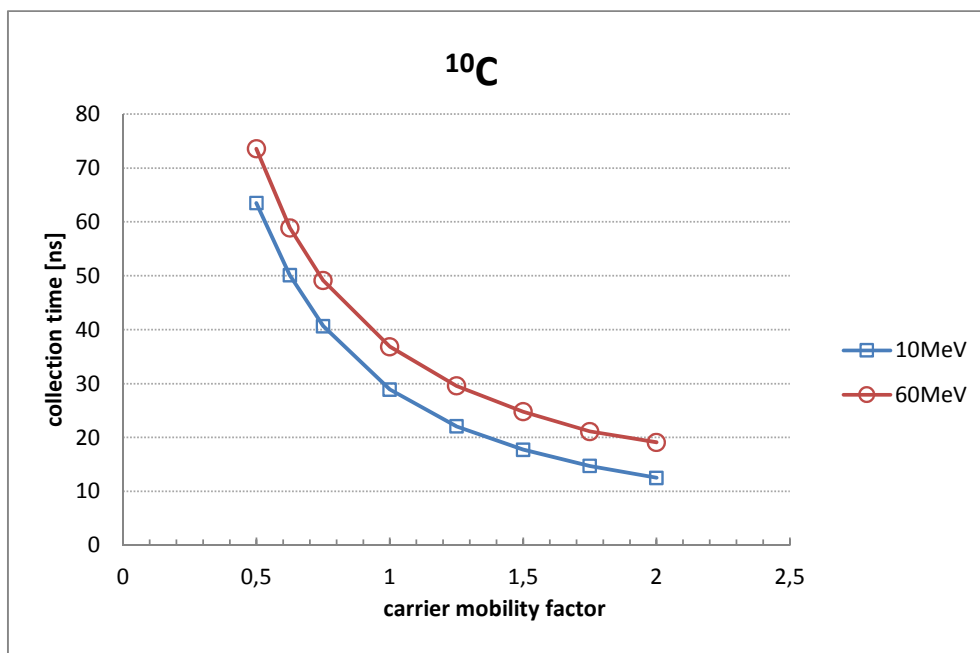


Figure 6.2: Correlation collection time vs. carriers mobilities calculated for ^{10}C at 10 and 60 MeV. Carrier mobility factor is the ratio of the mobilities comparing to base parameters (as in 6.1).

carrier energy exceeds the optical phonon energy, the probability of emitting an optical phonon also rises. This mechanism causes the carrier velocity to saturate with increasing electric field.

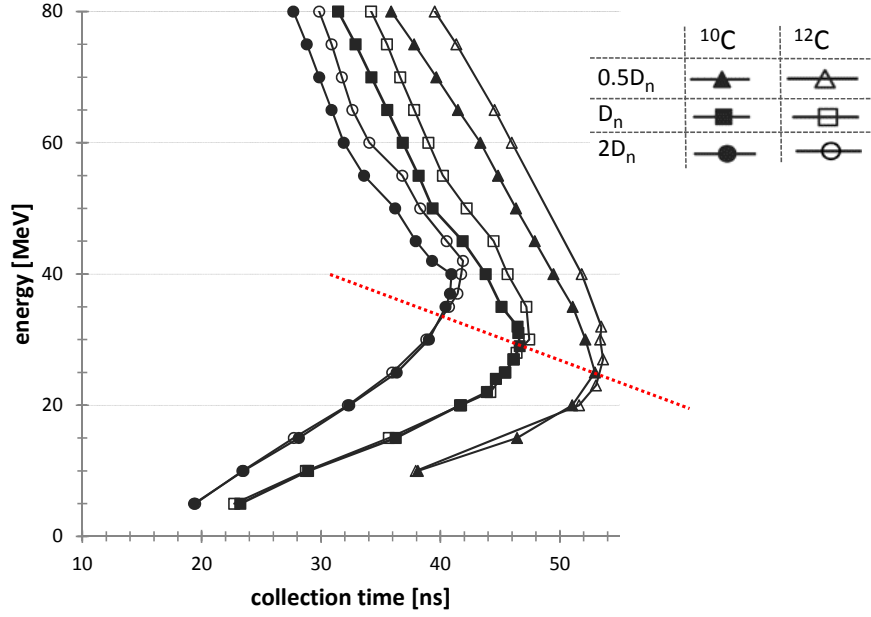


Figure 6.3: Evolution of charge carriers collection time with different diffusion coefficients - smaller values of diffusion coefficient make the back-bending point move to lower energies. D_n is the diffusion coefficient in typical conditions (detector properties as in 6.2).

This effect is further illustrated in Figure 6.4, where one can observe lowering of the collection times for increasing diffusion coefficients (data for reaction at 10 and 60 MeV).

6.3 Charge clouds propagation in the perpendicular direction

Charge cloud propagation in perpendicular direction to the external electric field is driven by Coulomb forces between electrons and holes, their diffusion

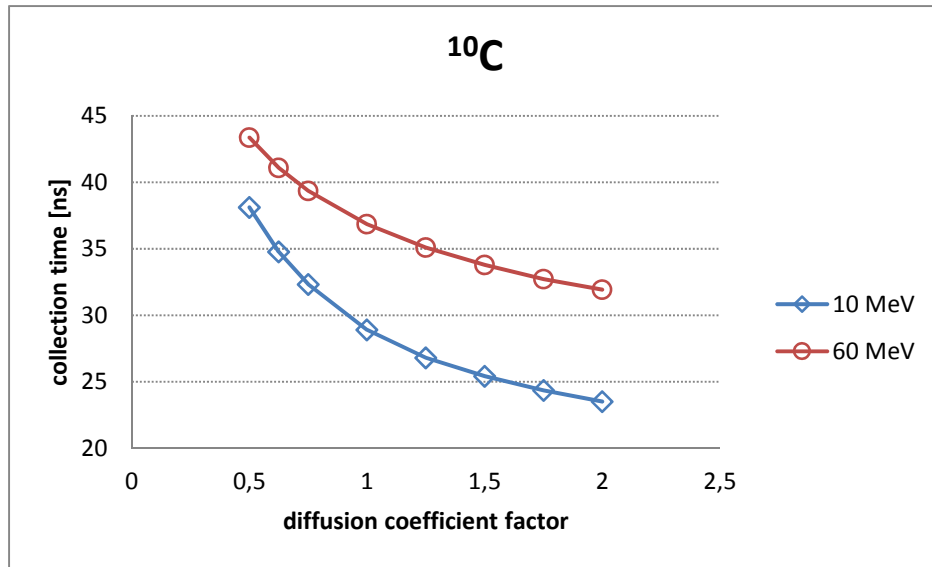


Figure 6.4: Correlation collection time vs. diffusion coefficients calculated for ^{10}C at 10 and 60 MeV. Diffusion coefficient factor is the ratio of the coefficient comparing to base parameter: $D_e = 3.49 \left[\frac{\mu\text{m}^2}{\text{ns}} \right]$.

and transport phenomena caused by gradients of densities of carriers. The rate of standard deviation expansion depends on the carriers mobilities in perpendicular direction, named in frames of the model [1] as electron or hole variance mobilities and on the diffusion coefficients of both carriers. The only free parameter of the model is electron variance mobility $\mu_{\sigma e}$ which is related to charge propagation in the perpendicular direction caused by Coulomb interaction solely. The respective variance mobility of holes $\mu_{\sigma h}$ was calculated using the model assumption of proportionality with the electron and hole standard mobilities along the external electric field direction:

$$\frac{\mu_{\sigma h}}{\mu_{\sigma e}} = \frac{\mu_{xh}}{\mu_{xe}} \quad (6.1)$$

It was checked how $\mu_{\sigma e}$ values can influence system behaviour. The calculations were performed for $\mu_{\sigma e} = 0.5, 2, 4 \left[\frac{\mu m^2}{V ns} \right]$. Results are presented in Figure 6.5 for the case of ^{10}C stopped in the detector characterized in Table 6.2.

As one can see, the back-bending point shifts to lower energies with increasing $\mu_{\sigma e}$. This means lowering of identification energy threshold for the PSA method. Cloud propagation in the direction perpendicular to the external electric field is driven by both diffusion and Coulomb forces. The contribution of the Coulomb component to this mechanism is demonstrated in Figures 6.6, 6.7, and 6.8. These diagrams present the evolution of the standard deviation of the charge distributions induced by ionization of ^{10}C particles with energy 60 MeV, stopped in a silicon detector characterized in 6.2. In these pictures, holes are collected at the right side of the overlap region and electrons at the left side.

We consider the situation where Coulomb forces between electrons and holes are gradually activated in the model. For $\mu_{\sigma e} = 0.5 \left[\frac{\mu m^2}{V ns} \right]$ (Figure 6.6) the propagation of electrons and holes is weakly influenced by their interactions and thus does not depend strongly on the position within the detector. Increasing of Coulomb forces changes the system evolution by the attraction forces between the clouds. In the overlapping area mutual interactions of carrier clouds slow down electrons propagation and speed up holes. This can be noticed in Figures 6.7 and 6.8 on panels presenting cloud variances evolution at instants $t = 5, 10, 15, 20$ and 25 ns.

Situation changes when hole and electron concentrations start to differ and Coulomb forces make perpendicular propagation faster. That can be noticed nearby electrode collecting electrons, close to $x \approx 0 \mu m$ where the motion towards electrode results in the increase of electron distribution width and similarly for holes close to $x \approx 310 \mu m$. Clouds are getting more dispersed, resulting in a weaker electron and hole charge interactions reducing

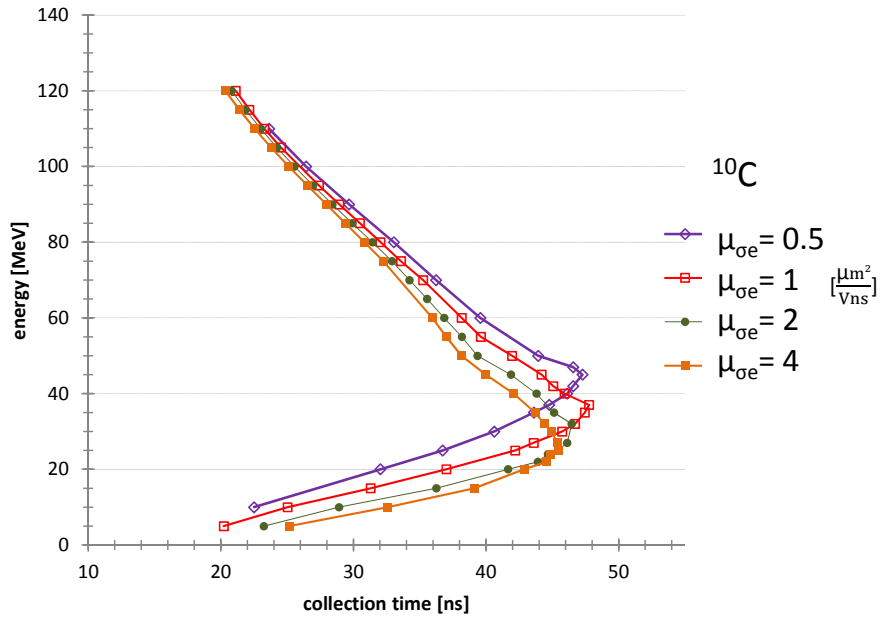


Figure 6.5: Dependence of PSA correlation shape on the carrier variance mobility (detector properties as in 6.2).

the Plasma Delay Effect. The low energy particles are stopped close to the entrance electrode due to the short range. Thus, the aforementioned PDE reduction is inversely proportional to the particle energy. The effect of increased dispersion of the charge is most pronounced for a short overlap area, close to the rear side collecting electrode. For higher energy, the charge cloud overlap starts to dominate ionization area and then PDE becomes stronger. For particles with energies above the threshold of identification, the majority of ionization falls into the strong external electric field region where Coulomb interactions between carrier clouds are of less importance for the charge collection process. Therefore, at higher energies one can observe shortening of collection times. As a result, correlation between carriers collection time and energy show familiar shape with back-bending point presented already e.g. in Figure 3.7.

6.4 Details of isotopic identification

As mentioned in Chapter 5, some new calculations were performed aiming at verifying the model response to the example of Boron and Carbon isotopes stopped in the example case of silicon detector. The simulations were done with the default parameter set (as in Table 6.1). Results are presented in Figures 5.1, 5.2. As one can see they nicely follow experimental trend with back-bending of identification curves at low energies. The comprehensive view on propagation for all the simulated isotopes is presented in Figure 6.9 which includes Boron isotopes ^{10}B , ^{12}B , ^{14}B and Carbon isotopes ^{10}C , ^{12}C , ^{14}C in one picture.

One can see that moving to low energy after passing the back-bending point, collection times are getting shorter all the more for the heavier isotopes. Figure 6.10 illustrates this behaviour by zooming in on the low energy region of the right panel from Figure 5.2 (for better clarity it shows only two Carbon isotopes: ^{10}C , ^{12}C).

Additionally we introduce tables presenting exact collection times in the region of low and high energy - Tables 6.3 and 6.4.

This 'inversion' may be explained by the following arguments: For initial equal kinetic energy E of both isotopes the ranges $R_{^{10}\text{C}}$ and $R_{^{12}\text{C}}$ in silicon detector are roughly related by the proportion of their masses:

$$R_{^{12}\text{C}} = \frac{10}{12} R_{^{10}\text{C}} < R_{^{10}\text{C}} \quad (6.2)$$

Above the back-bending energy the mean carrier density per track length

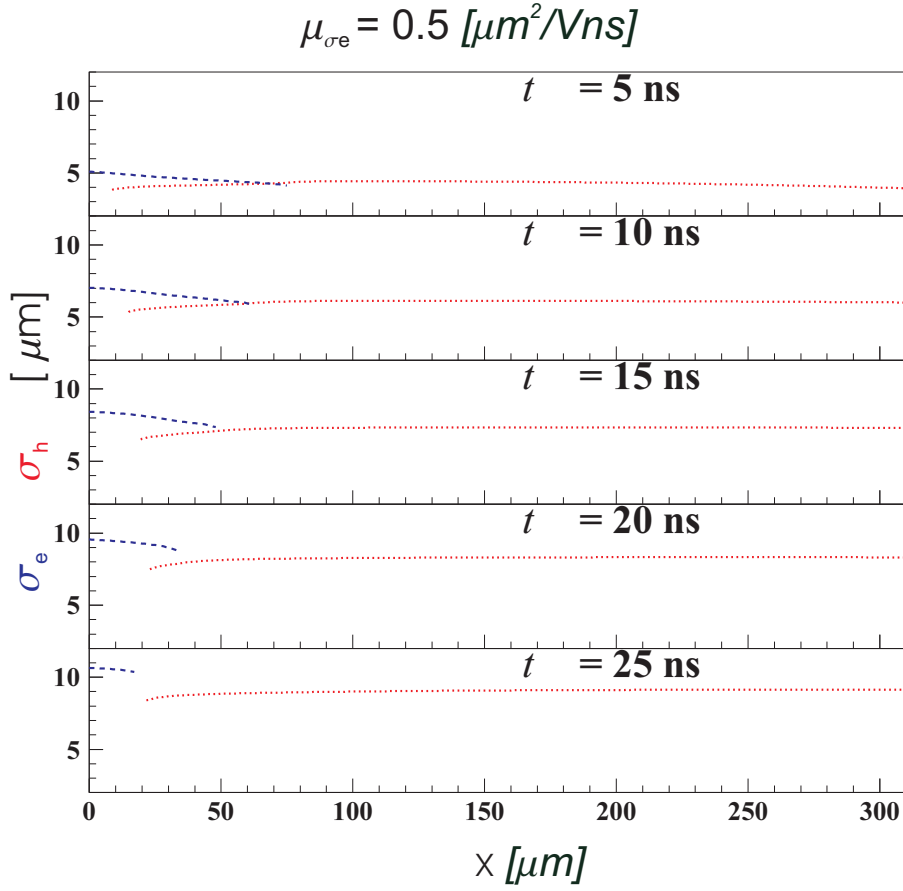


Figure 6.6: The evolution of the width of the charge distributions for $\mu_{\sigma e} = 0.5 [\frac{\mu m^2}{Vns}]$ at energy of 60 MeV. Calculations performed for ^{10}C ions at instants $t = 5, 10, 15, 20$, and 25 ns after full stopping in the silicon detector (detector properties as in 6.2). Standard deviations for electrons are represented by a dashed blue line and variances for the holes by a dotted red one.

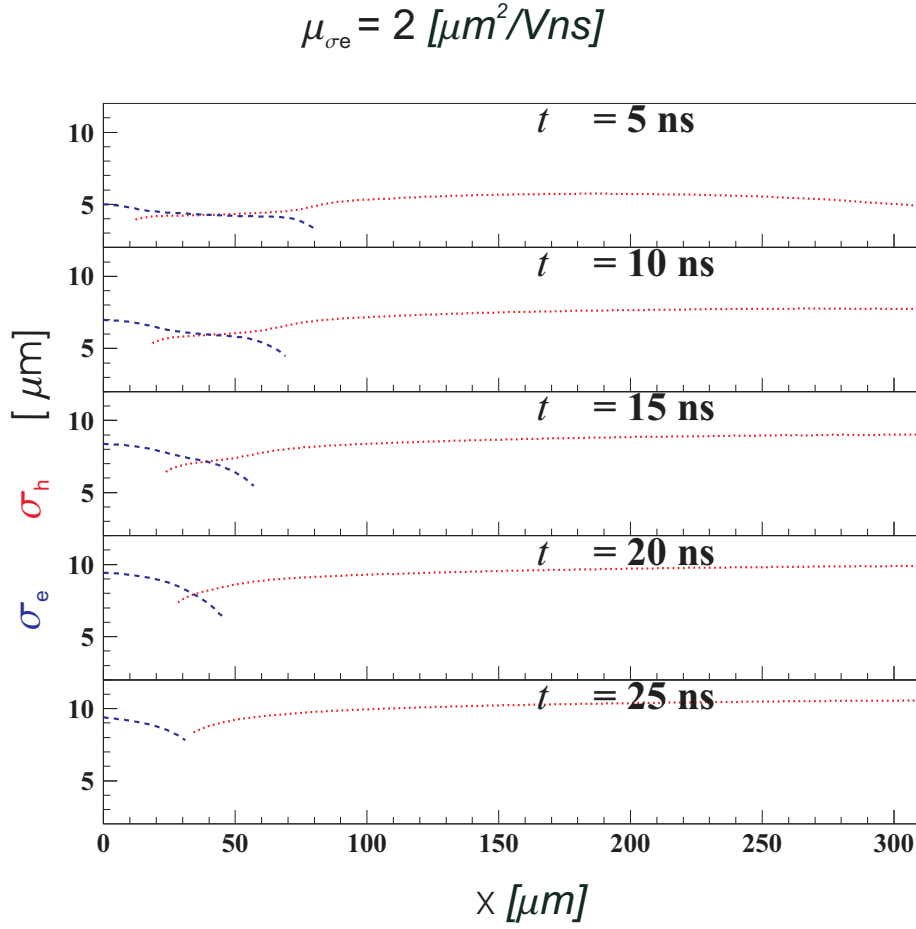


Figure 6.7: The evolution of the width of the charge distributions for $\mu_{\sigma e} = 2 \left[\frac{\mu m^2}{Vns} \right]$ at energy of 60 MeV. Calculations performed for ^{10}C ions at instants $t = 5, 10, 15, 20$, and 25 ns after full stopping in the silicon detector (detector properties as in 6.2). Standard deviations for electrons are represented by a dashed blue line and variances for the holes by a dotted red one.

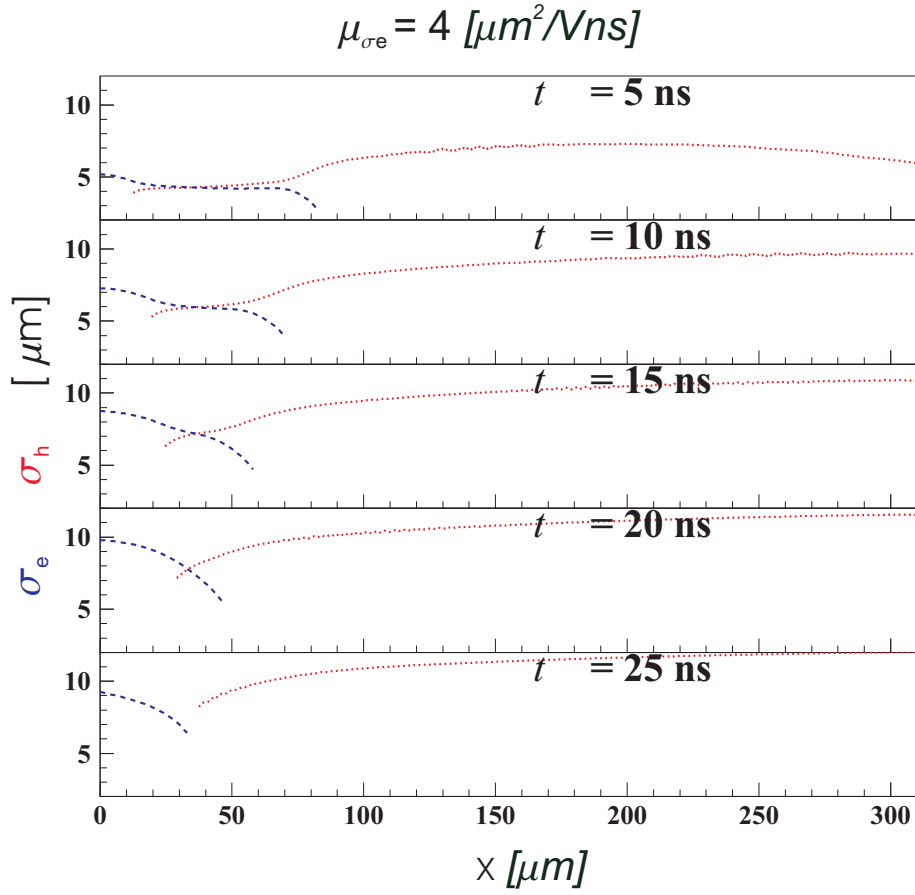


Figure 6.8: The evolution of the width of the charge distributions for $\mu_{\sigma e} = 4 \left[\frac{\mu m^2}{Vns} \right]$ at energy of 60 MeV. Calculations performed for ^{10}C ions at instants $t = 5, 10, 15, 20$, and 25 ns after full stopping in the same detector (detector properties as in 6.2). Standard deviations for electrons are represented by a dashed blue line and variances for the holes by a dotted red one.

Table 6.3: Collection times simulated for Carbon isotopes in lower energies (below the back-bending region)

Energy [MeV]	$t_{col}({}^{10}\text{C})$ [ns]	$t_{col}({}^{12}\text{C})$ [ns]
5.0	23.23	22.72
7.5	25.36	25.29
10.0	28.91	28.75
12.5	32.58	32.23
15.0	36.25	35.69
17.5	39.06	38.77

Table 6.4: Collection times simulated for Carbon isotopes in higher energies (above the back-bending region)

Energy [MeV]	$t_{col}({}^{10}\text{C})$ [ns]	$t_{col}({}^{12}\text{C})$ [ns]
50	39.34	42.21
55	38.17	40.21
60	36.84	39.00
65	35.56	37.80
70	34.22	36.63
75	32.90	35.53

prevails:

$$\frac{E}{R_{12C}} > \frac{E}{R_{10C}} \quad (6.3)$$

and hence the carrier collection times are longer for heavier isotope: $\tau_{12C} > \tau_{10C}$. Below the back-bending energy prevails the role of range close to the electrode entrance, $R_{12C} < R_{10C}$, and hence $\tau_{12C} < \tau_{10C}$. This effect of the competing factors is small but suggests some chance to improve isotopic resolution when used as supplementary information to the time of flight (TOF) method.

6.5 Mirror effects

The method of images [33] simplifies solving of electrostatic systems, where Green's function method is involved. This technique deals with a problem of one or more point charges in the presence of boundary surfaces. The boundary conditions are simulated by charges located externally to considered area. In case of model [1] it describes charges generated by a particle stopped in a detector as clouds interacting with their reflections related to electrodes (same variance, reverse charge, localised symmetrically to electrodes), which is visualised in Fig. 4.1 by solid line graphs.

Model approximation takes into account only the nearest mirror charges. In order to verify the impact of interactions of charge clouds with mirror reflections in electrodes, we have performed several calculations within the frame of the model. It seems that this interaction causes plasma to be less stable close to the electrodes while ionizations far from electrodes are determined by interaction between electron and hole clouds solely. In the model, only first-order mirror reflections in the electrodes were considered. Figure 6.11 presents that assumption: charge generated is treated as a cloud of maximum density located at x coordinate (solid line) interacting with reflections related to electrodes positioned at coordinate 0 of the entrance of the detector (of depth d). The same shape (e.g., variance) of the generated mirror charge is assumed. The second (dashed) and third (dotted) reflections are also presented. They will be included in the next model improvements as they are expected to influence charge carriers evolution especially for thinner detectors where respective distances are shorter.

In Figure 6.12, the influence of the mirror charges on the predictions of the model for Carbon and Boron for the detector of $310\mu m$ thickness is shown. Neglecting effects related to mirror charge reflections in the first order affects the identification correlation significantly, especially around back-bending energies. The influence of higher-order reflections is regularly decreasing;

therefore, the implementation of a convergent treatment is possible to include the infinite series of mirror reflections.

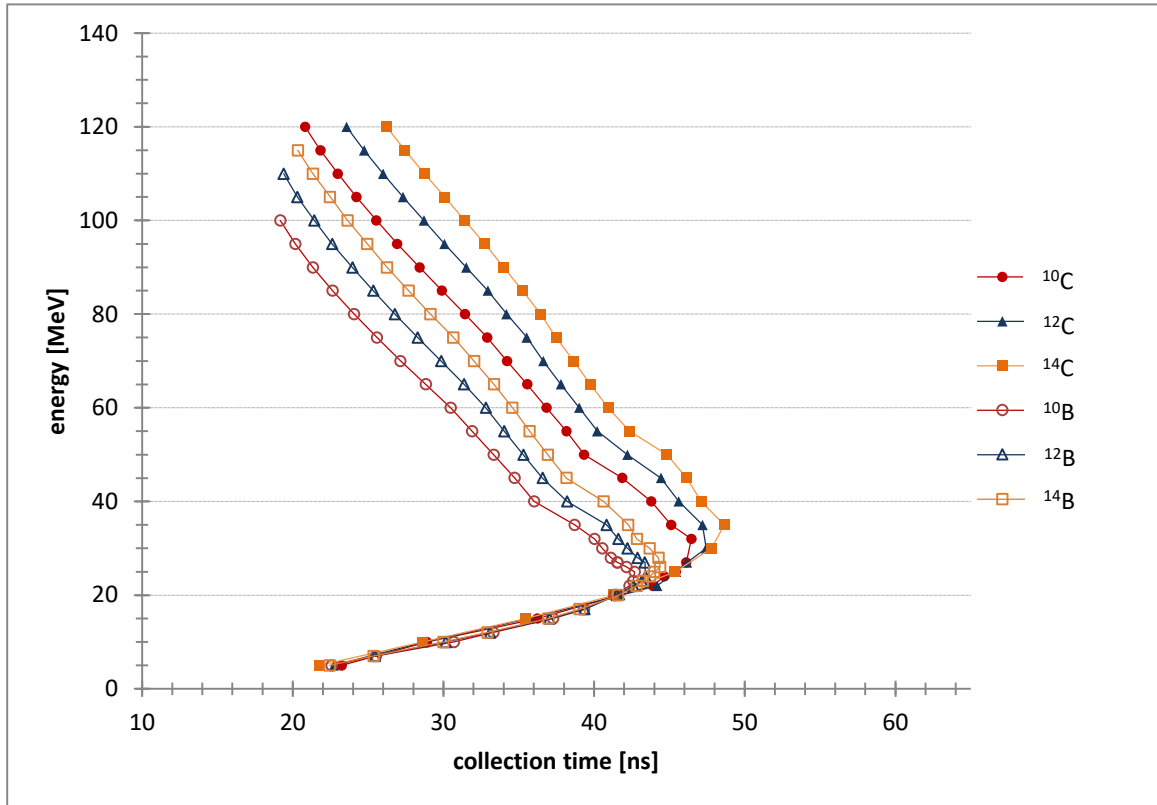


Figure 6.9: Model calculation for Boron isotopes ^{10}B , ^{12}B , ^{14}B and Carbon isotopes ^{10}C , ^{12}C , ^{14}C - energy versus collection time identification matrix (silicon detector: thickness $310\ \mu\text{m}$, $V = 190\text{V}$).

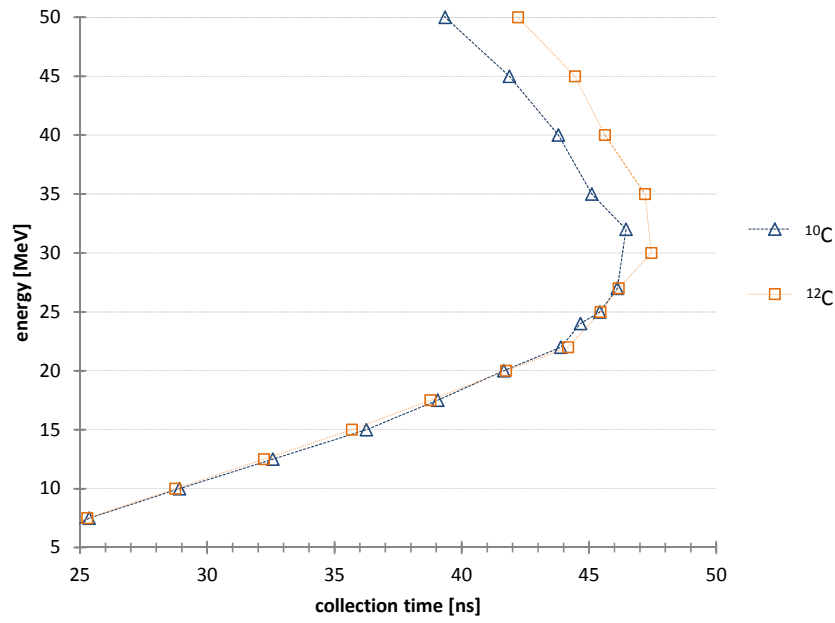


Figure 6.10: 'Inversion' in the region of back-bending point - calculation for Carbon isotopes (^{10}C , ^{12}C ; detector properties as in 6.2). For lower energies, collection times of heavier isotopes are getting shorter. Above the back-bending energies, one can observe the reversed relation - collection times of heavier isotopes become longer than those of lighter ones.

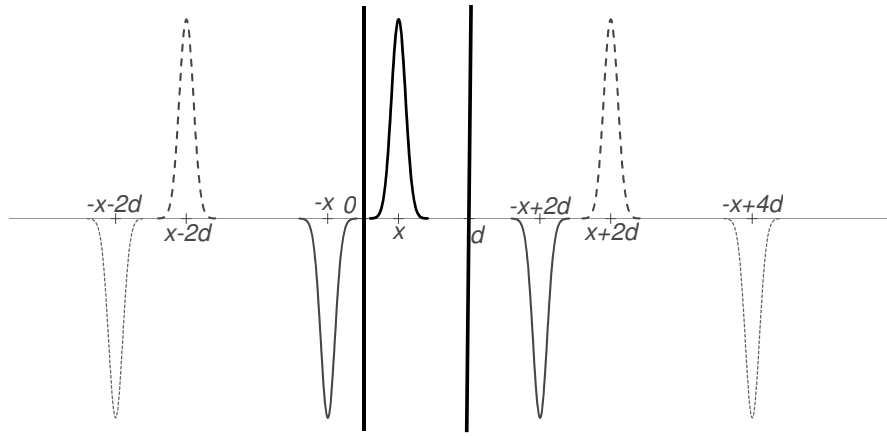


Figure 6.11: Charges generated by a particle stopped in a silicon detector are treated as clouds interacting with reflections related to electrodes positioned at 0 and d (same variance, reverse charge, localized symmetrically to electrodes). Only the nearest reflections are presently taken into account in the model. Second (dashed line) and third (dotted) mirror reflections are also presented; however, they are to be included in future model developments.

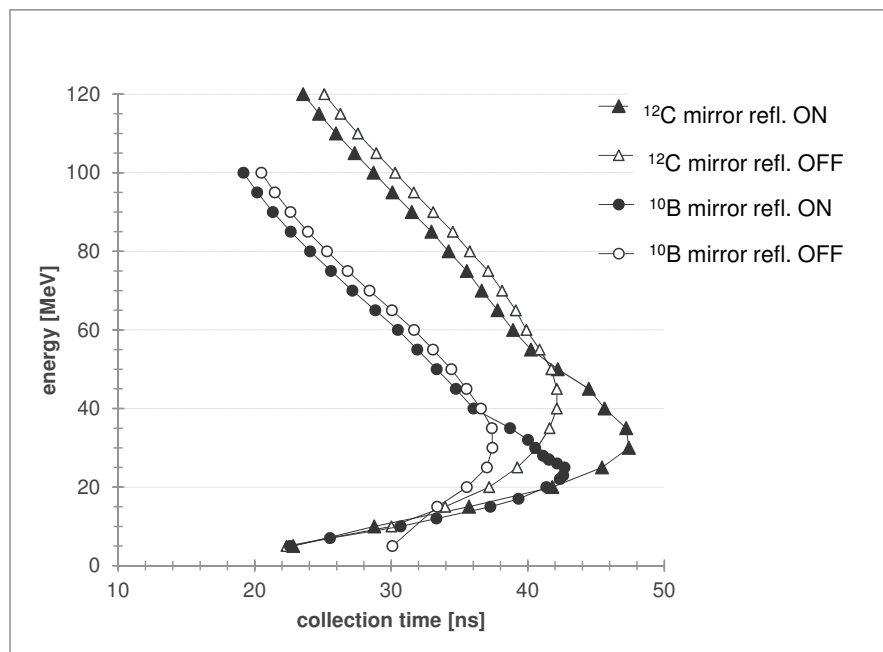


Figure 6.12: Evolution of charge carriers collection time with particle energy when mirror reflections are, or are not, taken into account in the model calculations.

Chapter 7

Reconstruction of the pulse shape

7.1 Ramo-Shockley theorem

In order to determine the induced charge on detector electrodes, the Ramo-Shockley theorem will be applied in our simulations.

Traditionally, before the 1930s, the resolution of Gauss's Law across various geometries at every coordinate was imperative for such analyses. However, a pivotal development occurred when Simon Ramo of General Electric and William Shockley of Bell Laboratories independently formulated a more efficacious methodology for the computation of induced charges and currents within vacuum tubes [34, 35]. The Ramo-Shockley theorem has become a fundamental principle in the fields of semiconductor physics and electronic engineering.

This approach introduces the methodology for calculating calculate the current generated by the motion of charged particles within a semiconductor. The configuration involving k electrodes, each assigned a specific voltage $V_1, \dots, V_k$ is considered. Utilising the principle of superposition, the overall potential $\Phi_0(\vec{r})$ in the space surrounding these electrodes can be modelled as the sum of individual potential contributions $\Phi_i(i=1, \dots, k)$. In each of these configurations, all electrodes are kept at zero potential except for the one electrode i being set to its respective voltage V_i . Figure 7.1 schematically illustrates the fundamental assumptions explained above.

Originally, Shockley and Ramo confined their research to a scenario with a single electron travelling through a vacuum near multiple conducting electrodes. It was presented that the instantaneous current on a particular electrode labelled i induced by an electron at the position $\vec{x}$ is described by the equation:

$$I_i = e\vec{v} \cdot \vec{E}_{wi}(\vec{x}) \quad (7.1)$$

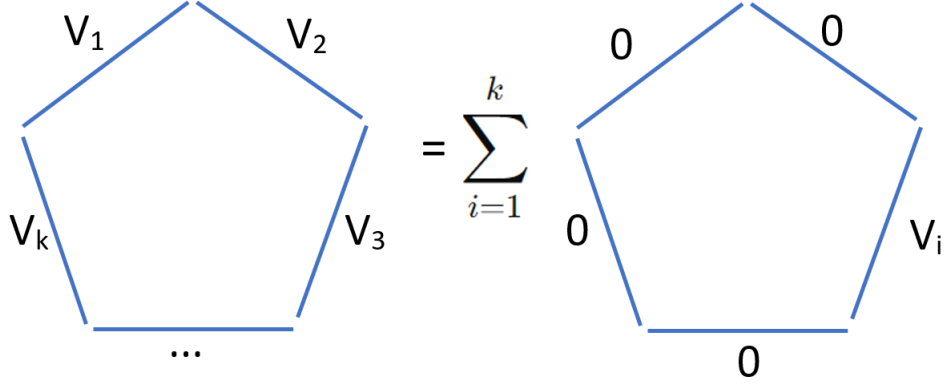


Figure 7.1: Schematic illustration of the fundamental assumptions used in the Ramo-Shockley theory. Figure adapted from [36] .

where $\vec{v}$ - instantaneous electron velocity, e - electron charge.

$\vec{E}_{wi}(\vec{x})$ is an electrode weighting field, characterized as the electric field at position $\vec{x}$, assuming all electrodes are grounded, except for electrode i (maintained at potential of 1 V).

Subsequently, it was generalised in [37] that the same result is obtained in the presence of multiple electrons within the device. Consequently, the total current is the aggregate of the currents induced by each individual electron.

7.2 Application of the theorem to the GCD model

To roughly estimate the pulse shape, we approximately characterize the partial current related to the Gaussian cloud. To simplify the calculations, we apply the Ramo–Shockley theorem and convert the Gaussian charge distribution to a point-like shape.

The results of the computational analysis are illustrated in Figures 7.2, 7.3, and 7.4. The aggregate current pulse is depicted as a solid black line,

while the contributions from electrons and holes are respectively represented by a blue line and a red line. The simulation runs were performed for ^{12}C at 80 MeV using three assumed values of electron variance mobility $\mu_{\sigma e} = 1, 2, 4 \left[\frac{\mu\text{m}^2}{\text{Vns}} \right]$.

Comparing these figures reveals that the main differences can be observed in the holes contribution, which impacts the total signal values. This is consistent with the previous statement about the simulation being dominated by the evolution of the holes.

Signal generation is strongly influenced by the front-end electronic device, preamplifier, as it is directly connected to the detector. Reconstruction of the pulse shape may be important in understanding of these crucial role in signal acquisition and may lead to some conclusions for future considerations or model enhancements. One of the important factors is a cutoff frequency ω_0 (unity gain frequency) which is strongly correlated with transistors characteristic and the electronic circuit geometry.

To simulate the response of the preamplifier electronics to the input current pulse, specialized software can be developed. This allows for the emulation of various scenarios and facilitates the analysis of the system behaviour under different conditions. For the purposes of qualitative observation we applied the approach introduced in [21].

Numerical modelling was conducted using the SPICE program (Simulation Program with Integrated Circuit Emphasis), a software designed for the analysis and design of electronic circuits. The primary purpose of SPICE is to allow engineers to predict the functionality of a circuit virtually before physical construction. This modelling is crucial in the design of both simple circuits and complex electronic systems, including integrated circuits.

The environment was originally developed at the University of California, Berkeley, in the 1970s and evolved into a comprehensive suite of software tools widely used for simulating electronic circuits.

Its capabilities include a variety of analyses, such as DC, AC, transient, and parametric analyses, allowing engineers to theoretically predict circuit behaviour. With support for a wide array of circuit elements, such as resistors, capacitors, transistors, and integrated circuits, SPICE facilitates the simulation of both analog and digital circuits.

SPICE is extensively applied across multiple domains, from microelectronics and telecommunications to power electronics and beyond, enabling engineers to iterate, optimize, and validate circuit designs with confidence and efficiency.

Figure 7.5 presents the calculation from Figures 7.2, 7.3, and 7.4 but after applying the preamplifier response function. This total signal visualization

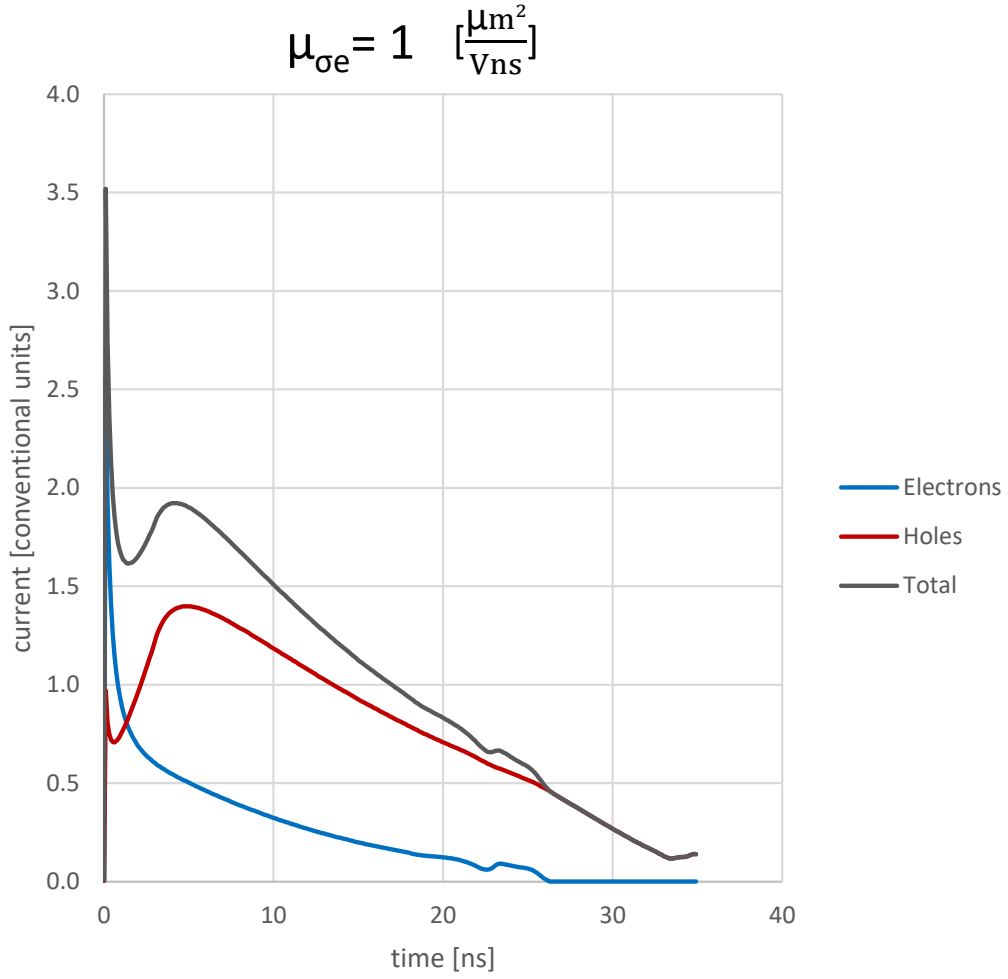


Figure 7.2: The model outcome of the current signal generated by 80 MeV ^{12}C ions entering the silicon detector. The results have not been adjusted for the preamplifier response. Model assumption: electron variance mobility $\mu_{\sigma e} = 1 \left[\frac{\mu m^2}{V ns} \right]$.

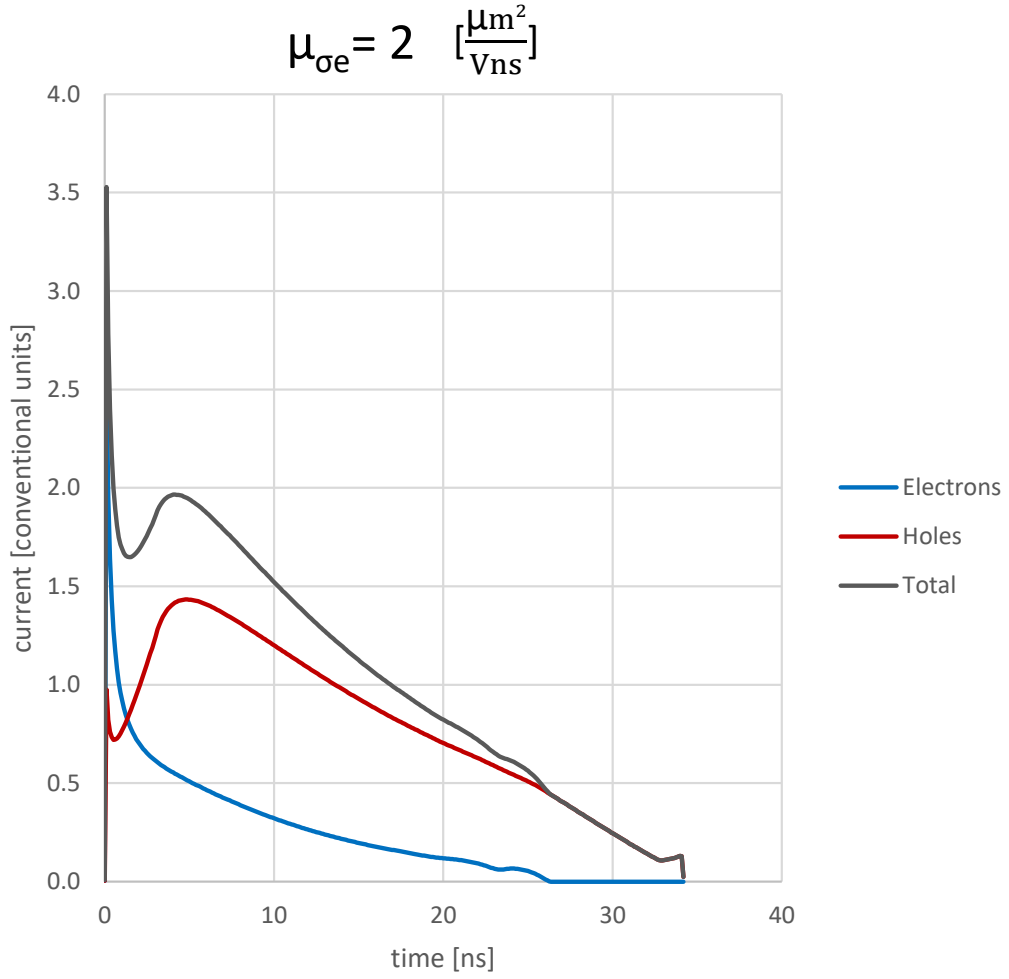


Figure 7.3: The model outcome of the current signal generated by 80 MeV ^{12}C ions entering the silicon detector. The results have not been adjusted for the preamplifier response. Model assumption: electron variance mobility $\mu_{\sigma e} = 2 \left[\frac{\mu m^2}{V ns} \right]$.

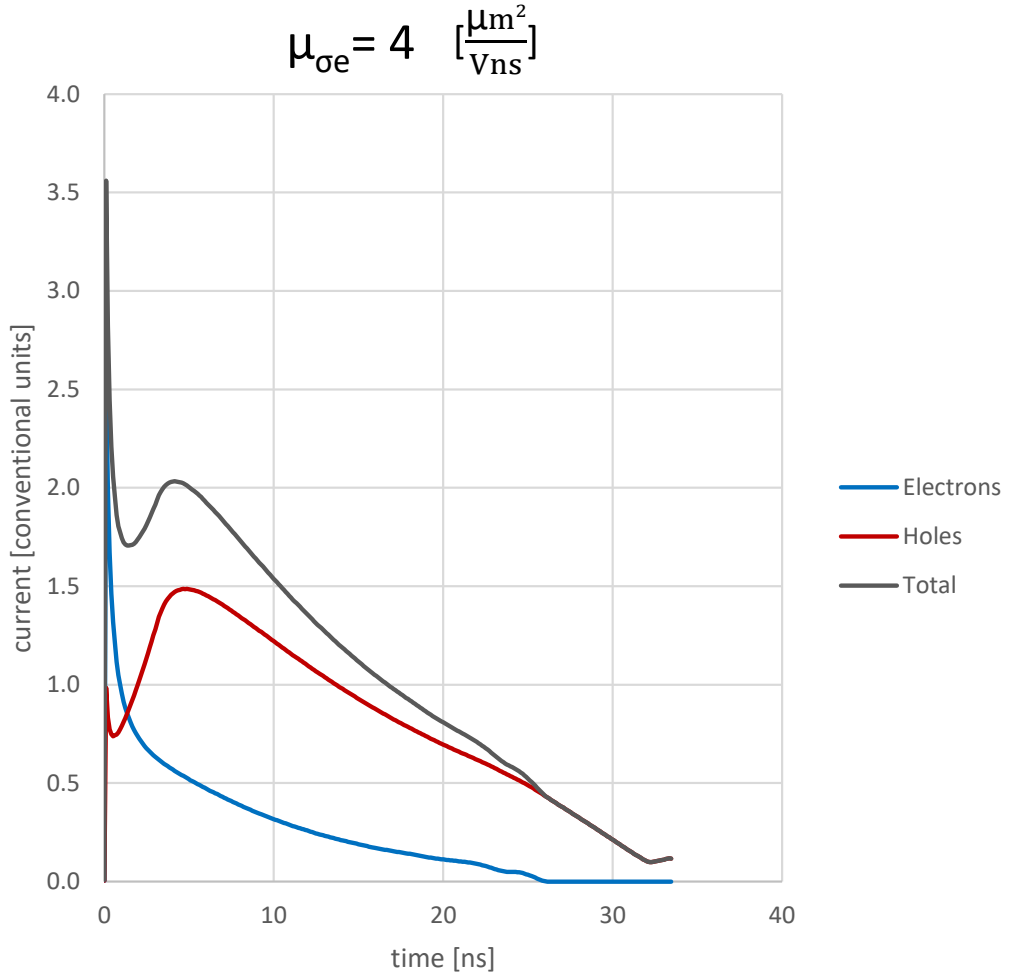


Figure 7.4: The model forecast of the current signal generated by 80 MeV ^{12}C ions entering the silicon detector. The results have not been adjusted for the preamplifier response. Model assumption: electron variance mobility $\mu_{\sigma e} = 4 \left[\frac{\mu m^2}{V ns} \right]$.

allows us to see the pulse shapes on a single diagram for all three assumed model values of electron variance mobility $\mu_{\sigma e} = 1, 2, 4 \left[\frac{\mu m^2}{V ns} \right]$.

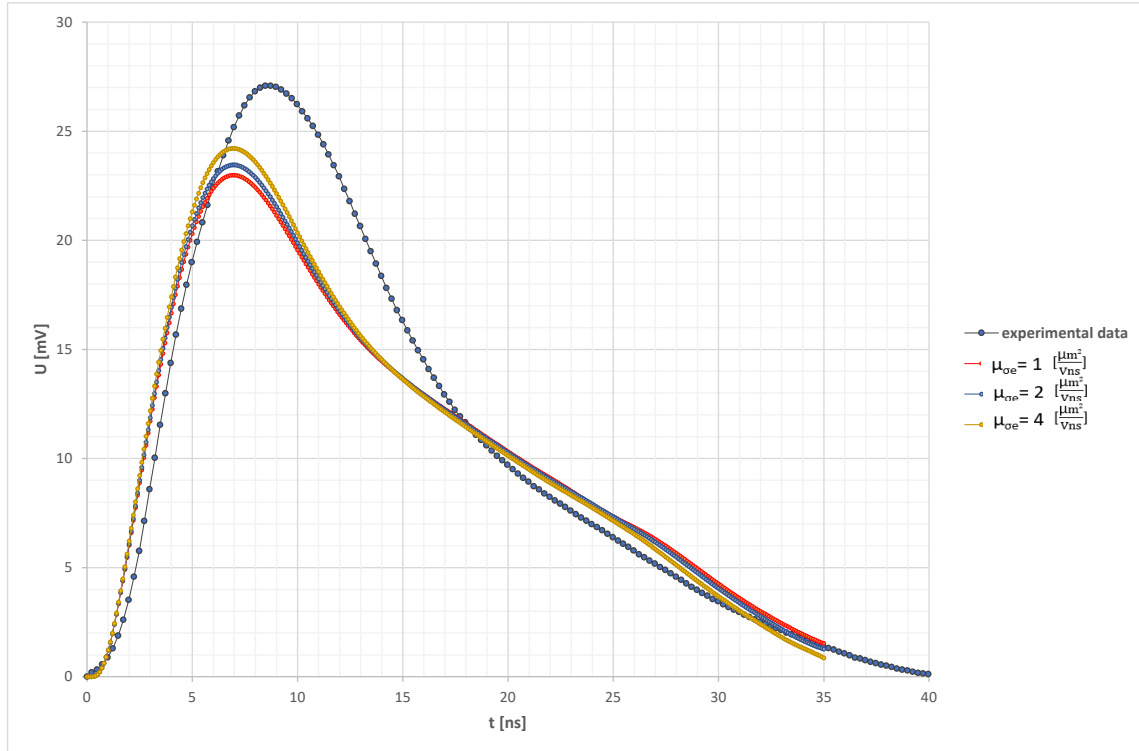


Figure 7.5: The model forecast of the current signal generated by an 80 MeV ^{12}C entering the silicon detector after applying the preamplifier response function. Model assumption: electron variance mobility $\mu_{\sigma e} = 1, 2, 4 \left[\frac{\mu m^2}{V ns} \right]$.

Chapter 8

Temperature impact on the carrier mobility

Current considerations were based on the fixed values of the carrier mobilities. All simulations so far were conducted for the following values: $\mu_{xe}=135 \left[\frac{\mu m^2}{V ns} \right]$; $\mu_{xh}=47.5 \left[\frac{\mu m^2}{V ns} \right]$. Correlation collection time-energy as a function of diffusion coefficient is presented in Figure 6.3, but this observation does not consider the temperature dependency on electrons and holes mobilities. That is essential in numerical simulations to have a solid modelling basis to present carriers mobilities as a function of parameters like temperature. Among a few approaches to these calculations, we focused on searching for empirical relationship between those factors. To modify the propagation model we used Arora mobility approach [38].

This research presents analytical formulas for the carriers mobilities. The obtained expressions allows to present electron and hole mobilities as a function of concentration in a temperature ranges 250-500 K. Those are derived from experimental data and the modifications to Brooks-Herring theoretical considerations [39]. Authors used for fitting the similar approach to what was published in [40], i.e. mobility μ is presented in following form:

$$\mu = \mu_{min} + \frac{\mu_0}{1 + \left(\frac{N}{N_{ref}} \right)^\alpha} \quad (8.1)$$

where μ_{min} - minimum mobility expected, μ_0 - difference between maximum and minimum mobility expected, N_{ref} - reference concentration, α - factor binding concentration with N_{ref} . For electron considerations, lattice scattering mobility μ_{Le} was fitted using

$$\mu_{Le} = 8.56 \cdot 10^8 T^{-2.33} \quad (8.2)$$

where T is a temperature in Kelvins. For calculations of ionized impurity scattering mobility μ_{Ie} was considered based on [39]:

$$\mu_{Ie} = \frac{7.3 \cdot 10^{17} T^{\frac{3}{2}}}{N_I G(b)} \quad (8.3)$$

where N_I - number of ionized impurity atoms and

$$b = \frac{1.52 \cdot 10^{15} T^2}{n(2 - \frac{n}{N})} \quad (8.4)$$

where n - electrons density (cm^{-3}) and the function $G(b)$:

$$G(b) = \ln(b+1) - \frac{b}{b+1} \quad (8.5)$$

These considerations lead to empirical expression presenting electron mobility as a function of concentration and temperature

$$\mu_{xe}(T, N) = 88 T_n^{-0.57} + \frac{7.4 \cdot 10^8 T^{-2.33}}{1 + [N/(1.26 \cdot 10^{17} T_n^{2.4})] 0.88 T_n^{-0.146}} \quad (8.6)$$

where $T_n = T/300$, N - dopant concentration. In case of holes calculations, lattice scattering mobility μ_{Lh} was considered as:

$$\mu_{Lh} = 1.58 \cdot 10^8 T^{-2.23} \quad (8.7)$$

and hole ionized scattering mobility μ_{Ih} reads:

$$\mu_{Ih} = \frac{5.6 \cdot 10^{17} T^{\frac{3}{2}}}{N_I G(b)} \quad (8.8)$$

where

$$b = \frac{2.5 \cdot 10^{15} T^2}{p(2 - \frac{p}{N})} \quad (8.9)$$

and p - hole density (cm^{-3}). Those assumptions come to empirical function presenting hole mobility as a function of concentration and temperature:

$$\mu_{xh}(T, N) = 54.3 T_n^{-0.57} + \frac{1.36 \cdot 10^8 T^{-2.23}}{1 + [N/(2.35 \cdot 10^{17} T_n^{2.4})] 0.88 T_n^{-0.146}} \quad (8.10)$$

These formulas can be visualized as shown in Figure 8.1, which illustrates the impact of temperature on electrons and holes mobility based on the Arora model [38].

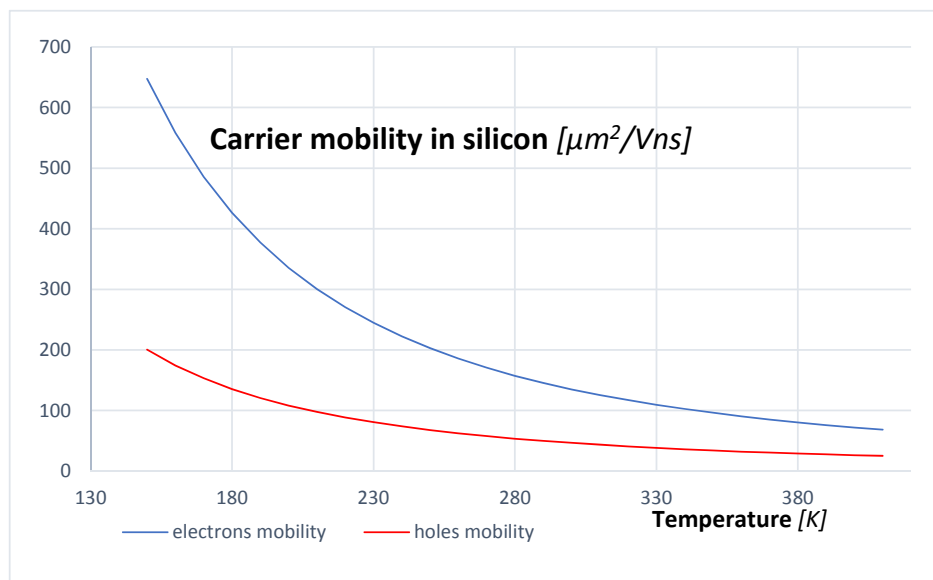


Figure 8.1: Impact of temperature on electrons and holes mobility - illustration based on Arora model.

This research highlights the need to examine the influence of lowering the temperature to determine if it slows the evolution of the system. A positive temperature factor on the diffusion coefficient might be dominated by increased values of the electrons and holes mobilities. The model calculations were conducted for ^{10}C isotope in the same detector system as before, with the temperature set to 270K and in the energy range of 10-105 MeV. The results are presented in Figure 8.2.

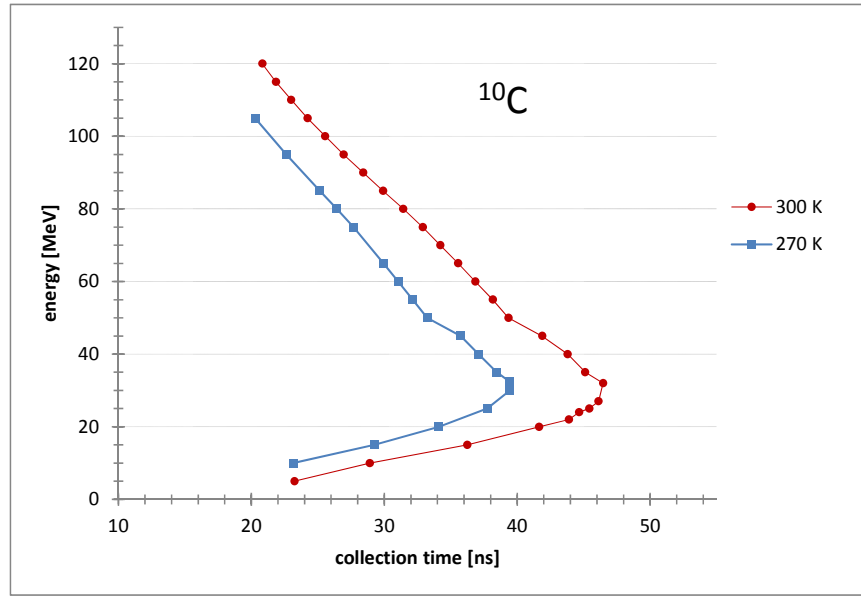


Figure 8.2: Comparison of collection time - energy correlation for different temperature values (270K, 300K) including impact on carriers mobility calculated based on [38]. Model simulation conducted for ^{10}C isotope in the energy range 10-105 MeV.

One can observe that the identification energy threshold is located around the same values, which does not improve the overall resolution ability. This leads to the conclusion that further material modification should be considered, such as dopant concentration adjustments. This may also open the need for researching other semiconductors (not so widely used) parameters to verify how the system evolution will be shaped at lower energies. The trend observation considering dopant concentration was visualized in Figure 8.3, where one can see how the electron mobility is dependent on the mentioned

concentration (shown for temperatures: 200K, 300K, 400K).

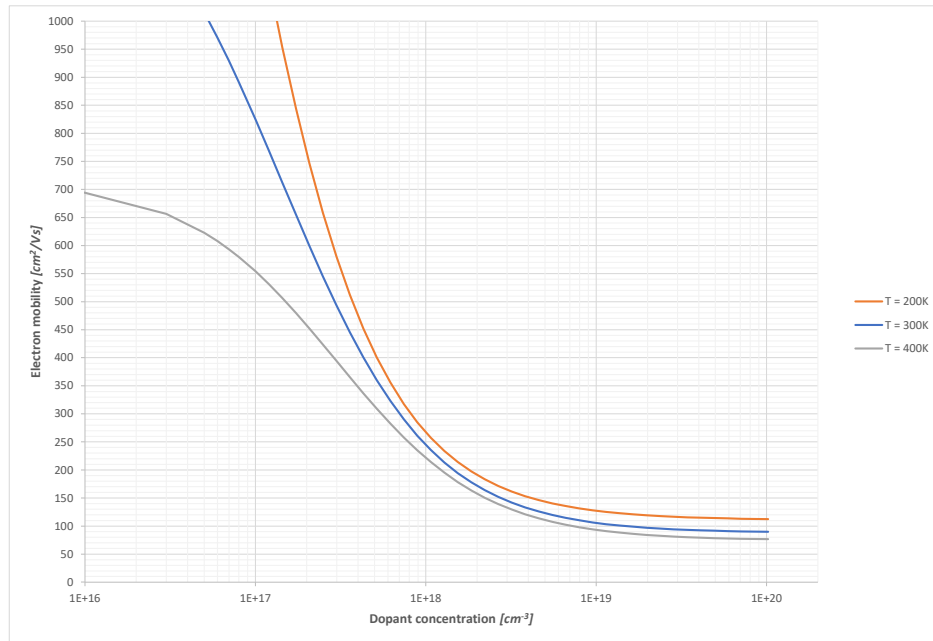


Figure 8.3: Visualization of formula 8.6: Electron mobility as a function of dopant concentration. Calculations were conducted for temperatures: 200K, 300K, 400K.

Chapter 9

Conclusions and perspectives

The microscopic Gaussian Clouds Dynamics (GCD) model was applied for the simulation of current pulse formation in silicon detectors, providing a theoretical understanding of Pulse Shape Analysis (PSA) techniques. This approach was based on the Ramo-Shockley theorem and accounted for Coulomb interaction between electron and hole clouds in the electric field of a depleted silicon detector. Several factors influencing the charge carriers collection process were investigated, including the Plasma Delay Effect, charge carriers mobilities, charge cloud variances, and mirror reflections in detector electrodes. Correlation matrices of charge collection time vs energy of the detected ions in silicon detectors were compared to model calculations for light isotopes, Carbon, and Boron. The model results qualitatively reproduced the correlation shapes obtained from experiments.

The discussion indicates the importance of seeking for detector characteristics that significantly improve identification ability. Additional considerations on temperature and doping dependency suggest that these factors may considerably influence system evolution. Further research into materials and modifications to achieve optimal characteristics, specifically investigating the lowest possible carrier mobility, should be considered.

To enhance the model accuracy, second and third mirror reflections should be included, as they impact plasma stability and may be required for a more reliable description of phenomena.

This research aims to enable calculations showing the impact of detector construction on particle identification, with some parameters being selectable and influenced by the experimental environment. Other aspects to consider include the case presented in [41], where effective isotopic identification via PSA has been achieved with a partially depleted detector, despite its doping uniformity being insufficient for isotopic identification at full depletion. This

factor opens another promising area for future model enhancements.

The software implementation of the GCD model is crucial for simulating detector responses and analysing experimental data. Continuous development and optimization are essential to keep pace with advancements in detector technology and computational methods. This PhD dissertation also proposes directions for these enhancements.

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