Simulation of a Fast Timing Micro-Pattern Gaseous Detector for TOF-PET and future accelerators

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Abstract. Simulation is a powerful tool for designing new detectors and guide the construction of new prototypes. Advances in photolithography and micro-electronics led to the development of a new family of devices named Micro-Pattern Gas Detectors (MPGDs) [1], with main features: flexible geometry; high rate capability ($> \text{MHz/cm}^2$); excellent spatial resolution ($< 100 \mu\text{m}$); good time resolution (5-10 ns); and reduced radiation length. A new detector layout, named Fast Timing MPGD (FTM), has been recently proposed [2] that would combine both the high spatial resolution and high rate capability of the MPGDs, while improving the time resolution with nearly two orders of magnitude to $\sim 100 \text{ ps}$. However charged particle timing with gaseous detector time resolution below 100 ps has been established with another detection scheme [3], this approach might not be able to sustain high particle rates. This contribution investigates the use of the FTM technology for an innovative TOF-PET imaging detector and emphasizes the importance of full detector simulation to guide the design of the detector geometry and performance.

1 Fast timing micro-pattern gas detector

Recently, a multi-layered detector with alternating drift and gain regions and resistive electrodes has been proposed [2]. In the drift region primary electron-ion pairs are created along the path of a charged particle passing through the detector, and they drift (due to a moderate electric field) to the gain region, where these primary electrons are multiplied and a detectable electric signal is created. The signals from each multiplication stage are read by the external readout electrodes through capacitive coupling. The time resolution of those Fast Timing MPGD (FTM) is governed by fluctuations in the distance between the closest electron-ion pair and the gain region and is improved reducing the drift distance of the closest primary electron by having several drift regions competing with each other, where the fastest drift time determines the time resolution.

Figure 1 (left) illustrates a 2-layer structure of the FTM. Not shown is the top cathode plane made of a polyimide foil covered with $\sim 100 \text{ nm}$ of Diamond Like Carbon (DLC). The coverlay spacers (red) of $250 \mu\text{m}$ height separate anode and cathode and define the drift gap. The amplification structure then consists of a polyimide foil of $50 \mu\text{m}$ height, covered also with DLC. This foil is mounted on top of a polyimide layer with both top and bottom covered with DLC. The top DLC electrode is connected to ground and serves to induce a high

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Figure 1. Illustration of a 2-layer FTM (with missing top electrode, left) and two possible detector schemes for the detection of 511 keV photons (right).

electric field inside the hole, while the bottom DLC coating serves as the cathode electrode for the next FTM layer. With top holes of $50\,\mu\text{m}$ and bottom holes of $70\,\mu\text{m}$ diameter spaced $140\,\mu\text{m}$ apart, which are the standard diameters and hole-spacing for GEM technology, a gain of ~ 5000 should be reachable in $\text{Ar}:\text{CO}_2$ (70:30) putting the anode at 500 V (100 kV/cm amplification field) and cathode at 575 V (3 kV/cm drift field).

2 Fast timing micro-pattern gas detectors for TOF-PET

Positron Emission Tomography (PET) is an imaging technique used to visualize organ and tissue functions. A positron-emitting radio nuclide (tracer) inside a biologically active molecule concentrates in tissues with high metabolic activity. The tracer undergoes β^+ decay, producing a positron that will annihilate (within $\sim 1\text{ mm}$ from the emission point) with an electron. This e^+e^- annihilation produces two back-to-back photons with energy of 511 keV. The detection of two coincident 511 keV photons allows to reconstruct a straight line (line of response, LOR), along which the annihilation took place. The measurement of several hundreds of thousands of LORs allows to reconstruct the concentration of the tracer.

In Positron Emission Tomography (PET) the quality of the reconstructed images can be improved when time-of-flight (TOF) information is used by reducing the zone of the positron emission to a fraction of the length of the Line of Response, leading to a higher contrast image and more accurate diagnoses [4]. The fine time resolution also allows to constrain the coincidence window for the two photons to be detected, leading to lower background.

Modified FTM detector layers specialized for TOF-PET are under study to optimize their ability to detect of 511 keV photons from positron annihilation. Two preliminary detector schemes are presented in Figure 1 (right): Scheme A where the photon converts in a dedicated layer and there is competition in two or more active area layers in order to optimize the time resolution; Scheme B where the amplification layer is made of material with high photon conversion efficiency in order to optimize the detection efficiency. Both schemes rely on the Compton scattering process to liberate an electron in a converter material with enough kinetic energy to reach the sensitive gaseous volume of the detector. For this reason, no energy measurement can be made. Using ADC counts or cluster counting low enenergy background electrons can be discriminated from hard Compton electrons with $50 < E < 350\text{ keV}$ of kinetic energy.

Figure 2. Interaction of a 511 keV photon in different materials, showing the normalised electron production rate (dashed lines) and escape rate as function of the material thickness.

3 GEANT4 simulations for photon detection

Electrons produced by the conversion of photons in the thin amplification layers are simulated using GEANT 4 version 10.03 [6–8]. The physics list considered is FTFP_BERT_LIV. Figure 2 (dashed lines) shows the photon conversion rate for different materials (kapton, FR4, glass, and lead glass) as function of the thickness (25 μm to 2 mm). We use GEANT 4 materials G4_KAPTON, G4_GLASS_PLATE and G4_GLASS_LEAD to define kapton, glass, and lead glass. FR4 (common PCB material) definition is implemented as 47.2% Epoxy and 53.8% SiO_2 . Electrons produced by photo-conversion can loose energy traversing the converter material and can be stopped instead of reaching the gas. The rate of electron escaping the material thickness is shown in figure 2 (solid lines). One can observe that for each material the exiting rate saturates, where the higher probability for photon conversion is mitigated by a lower exit probability for early conversions. We consider the thinnest material to reach this plateau as the optimum thickness: e.g. 100 μm for lead glass, resulting in a $\sim 3\%$ efficiency. For glass, FR4 and kapton the maximum efficiency is $\sim 2\%$ for materials of 300 ÷ 500 μm thickness. Assuming Scheme B, a single stack (1mm) could consist of 300 μm FR4 and 700 μm gas. Hundred of such stacks would lead to a detector with thickness of only 10 cm and detection efficiency of 20%. An upper limit to the efficiency of the conversion layer in this scheme would be 40% (photon interaction rate of $\sim 5\%$ divided by the electron exit rate of $\sim 2\%$).

The energy spectrum of the electrons in the drift region is shown in Figure 3 (left column) and can be used as input for the simulation of the primary ionization in the drift region and the avalanche in the gain region. The production energy at the moment of the photon conversion is shown in Figure 3 (right column) for the optimum thickness as defined earlier (all electrons: solid grey line, electrons reaching the gas: dashed grey line), together with the energy at the moment the electron escapes the material (colored solid line). Only the electrons with highest production energy can reach the gas while illustrating also the energy loss in the material.

4 Simulation of primary ionization and time resolution estimation

The 511 keV photon liberates a Compton electron and upon arrival in the gas this electron will ionize the gas and the liberated ionization electrons will drift towards the amplifica-

Figure 3. Electron energy distributions for (from top to bottom) kapton, FR4 and lead glass. The left figure shows the energy distribution of the electrons exiting different material thicknesses, while the right figure shows for a fixed thickness the kinetic energy at the production vertex for all electrons produced (solid grey line) and the subset of electrons escaping the material (dashed grey line), while the colored solid line shows the kinetic energy of the electron when entering the gas layer.

tion structure where they will be multiplied in an intense electric field, leading to a signal being picked up by external readout elements. The ionization pattern in the gas will determine the efficiency and time resolution of the signal. We have studied the primary ionization with two different codes: HEED [9] and Garfield++ Microscopic Tracking [10]. HEED implements the Photo-absorption ionization (PAI) model, splitting the atomic photoabsorption cross-section into partial cross sections for each subshell allowing in this way for atomic relaxation effects. As such the program allows for a detailed simulation of the primary ionization clusters along the trajectory of the original particle. Microscopic Tracking implements a rigorous tracking of the particle and all its daughter particles in the gas, sampling collisions with the gas molecules using the MAGBOLTZ [11] cross sections for elastic and inelastic collisions and excitation, ionization and attachment encounters. This method was originally

Figure 4. Mass stopping power in a gas mixture of Ar:CO₂ 70:30 (left) and Cluster density (right) simulated by HEED (open circles) and Microscopic Tracking (full circles) confronted with NIST ESTAR data (grey full circles and dashed line) and Bethe-Bloch calculations (green open circles and dashed line).

implemented for the simulation of avalanches where the mean electron energy rarely exceeds a few hundred eV and has shown to provide reliable results in this energy range [12].

The simulations were validated against NIST ESTAR data for the energy loss in Ar:CO₂ 70:30 gas mixture. Figure 4 (left) shows the good agreement between Bethe-Bloch calculations, NIST ESTAR data and HEED over the energy range 50-500 keV. Microscopic Tracking has good agreement up to ~100 keV above which it under estimates the energy lost in the gas, unable to reproduce the energy loss for a minimum ionising particle. Figure 4 (right) shows the number of clusters created by the ionizing particle along its trajectory. Here again, the ionization predicted by the Microscopic Tracking technique is slightly below the HEED prediction. As a cross check, we estimated the cluster density from theoretical Energy Loss calculations (Bethe-Bloch) by dividing with the average energy to create a *primary* ionization (W^{prim}) in Ar:CO₂ (70:30). W^{prim} was estimated by confronting the energy loss in pure Ar and CO₂ at minimum ionising energy ($\beta\gamma = 3.5$) with precise measurements of the specific primary ionisation 2.3 cls/mm for Ar and 3.4 cls/mm for CO₂ [13] and applying *Bragg's rule*, resulting in $W^{\text{prim}} = 103.7$ eV and 2.66 cls/mm for Ar:CO₂ (70:30). Another estimate of the cluster density was performed by inverting the mean free path for primary ionization: $N\text{Cls}/\text{mm} = \lambda_I^{-1} = (N\sigma_I)^{-1}$, using the weighted sum of the gross ionization cross section of electrons on Argon and electrons on Carbondioxide, extracted from MAGBOLTZ. From both plots we can conclude that HEED has the best performance for the simulation of energy loss and the simulation of primary ionization. Moreover, one can observe also that the curves of mass stopping power and cluster density have a similar logarithmic behaviour. Plotting HEED dE/dx vs NCls/mm and applying this correction to the NIST dE/dx , a NCls/mm estimate based upon NIST data was obtained and shown in Figure 4 (right).

The time resolution for a MPGD detector is determined by the drift velocity (v_d) of the electrons in the gas and the fluctuations of the distance of the closest electron to the amplification structure. The latter is given by the cluster density calculated earlier (Figure 4), while the former can be extracted from simple MAGBOLTZ simulations and is shown in Figure 5 (left). The occurrence of ionisation clusters is a Poisson process and therefore the distance d of the first ionisation cluster to the amplification structure follows an exponential distribution. The arrival time is given by: $t = d/v_d$ and the time resolution is given by: $\sigma_t = \sigma_d/v_d = \eta/v_d$, with η the cluster density ($\eta = N\text{Cls}/\text{mm} = \lambda_I^{-1}$), shown in Figure 5 (middle). Due to the high ionisation density, an electron of 50 keV kinetic energy can be detected with a time resolution

Figure 5. Left: Drift velocity as function of applied electric field in Ar:CO₂ 70:30 gas mixture. Middle: estimated time resolution as function of electron kinetic energy for a single gas layer in Ar:CO₂ 70:30 gas mixture and 3 kV/cm drift field. Right: CSDA range of electrons in various materials.

of nearly 1 ns, while 100 keV and 350 keV electrons will have at best a time resolution of 2 and 4 ns respectively when detected in a single layer. Better time resolutions can be obtained by the FTM principle dividing the drift region (cfr. Figure 1). If the Compton electron is energetic enough to penetrate through several amplification structures, the fastest signal will then determine the detector time resolution. Using CSDA ranges from NIST, shown in Figure 5 (right), one can estimate that a 350 keV electron can penetrate at least 8 layers of 100 μm kapton, giving signal in 9 layers and leading to a time resolution of 4 ns/9 = 0.45 ns, while a 100 keV electron could about just penetrate 100 μm kapton, leading to signals in two layers and a time resolution of 2 ns/2 = 1 ns. The time resolutions might however be better, since if a very soft (< 50 keV), the time resolution will be defined by the ionization in this layer. The time resolution might be further improved investigating gases and conditions (e.g. pressure) to increase the specific primary ionization and optimizing the material thicknesses.

5 Avalanche development

For the amplification structure of this detector we study the inverted cone geometry (50 μm top hole diameter and 70 μm bottom hole diameter) of the Fast Timing MPGD, determined by the etching procedure for the DLC coated polyimide. Figure 6 (left) shows the electric field simulated with COMSOL in a single layer, with the anode at 500 V (100 kV/cm amplification field) and cathode at 575 V (3 kV/cm drift field).

The electric field was simulated both with COMSOL and ANSYS. Figure 6 (right) demonstrates good agreement was found between the two Finite Element packages. A quick estimation of the gain was obtained by integrating the extracted effective Townsend coefficient from Magboltz (with a correcting for the Penning effect [14, 15]) along a line in the center of the hole:

$$G = \exp \int_0^h \alpha_{\text{Pen}} [E(z)] dz, \quad \alpha_{\text{Pen}} := \alpha \left(1 + r_{\text{Pen}} \frac{f^{\text{exc}}}{f^{\text{ion}}} \right)$$

with f^{ion} the direct ionization rate, f^{exc} the production rate of the excited argon states that can ionise CO₂ and r_{Pen} the Penning transfer rate, i.e. the probability that an excited Ar atom ionizes a CO₂ molecule. This method was cross-checked by estimating the gain observed in a similar wet-etched polyimide based detector [16] and good agreement was observed. A full Microscopic Tracking simulation was performed in Garfield++ simulating the avalanche induced by a single electron in the drift gap. The charge distribution obtained with Garfield++

Figure 6. Simulation of the electric field (V/m) in a single layer consisting of 250 μm drift gap and 50 μm high amplification structure with 50 μm top hole diameter and 70 μm bottom hole diameter and 140 μm pitch (140/50/70) (left). Confrontation of the electric field (kV/cm) simulated with COMSOL (solid line) and ANSYS (dashed line) for a the same structure, but now with top hole diameter 70 μm and bottom hole diameter 50 μm (140/70/50) (right).

Figure 7. Charge distributions simulated with Garfield++ for 100 kV/cm (left) and comparison between Gain simulated with Garfield++ and estimated with COMSOL (right).

with amplification field at 100 kV/cm and drift field at 3 kV/cm is shown in Figure 7 (left). The observed spectrum is fitted with a Polya distribution, Figure 7 (right) shows the agreement between the gain estimated with COMSOL and simulated with Garfield++. Perfect agreement is obtained when the Penning effect is not taken into account, a small difference however occurs when corrections for the Penning effect are taken into account.

6 Conclusion

Monte Carlo simulations are ubiquitous tools in the development of particle detectors, on the one hand to optimize the detector design, on the other hand to perform a feasibility study. In this paper two proposals have been presented for the detection of 511 keV photons. The photon conversion rate has been simulated with the GEANT 4 toolkit, while a time resolution estimation was derived from the simulation of primary ionization with HEED. Electric fields simulated with ANSYS and COMSOL show good agreement, while detector gains were obtained with Garfield. A feasibility study to adopt the FTM concept to reduce the time resolution to Compton-electrons from 511 keV photons was presented. We show that the use

of multiple detection layers could lead to a time resolution of 0.5 ns, to improve further on the time resolution, more detailed simulations are required, optimizing primary ionization and material thicknesses.

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