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

David Krapohl, Börje Norlin, Erik Fröjdh, Göran Thungström, Christer Fröjdh,

***Abstract*—X-ray imaging with spectral resolution, "Color X-ray imaging" is a new imaging technology that is currently attracting a lot of attention. It has however been observed that the quality of spectral response is degraded as the pixel size is reduced. This is an effect of charge sharing where the signal from a photon absorbed close to the border between two pixels is shared between pixels. This effect is caused by both diffusion during the charge transport and X-ray fluorescence in heavy detector materials [1]. In order to understand the behavior of pixellated detectors with heavy detector materials operating in single photon processing mode, we have simulated the X-ray interaction with the sensor and the transport of the charge to the readout electrode using a Monte Carlo model for the X-ray interaction and a drift diffusion model for the charge transport. By combining these models, both signal and noise properties of the detector can be simulated.**

***Index Terms*—x-ray, spectral resolution, Monte Carlo simulation, Geant4, TCAD**

I. Introduction

Color X-ray imaging is an emerging technology that attracts a lot of attention. However, charge sharing between pixels can reduce the spectral response. It is therefore important to develop models for heavy detector materials and study charge transport and X-ray fluorescence. We combined a Monte Carlo model implemented in Geant4 with drift diffusion model in the TCAD application Medici in a similar approach as described in [2], [3]. Python scripts were used to transfer data, create simulation scripts and convert units between both programs.

II. Methods

A. Monte Carlo Simulation

A Monte Carlo simulation of a part of the detector with dimensions of $10\,\mathrm{mm} \times 10\,\mathrm{mm} \times 1\,\mathrm{mm}$ was implemented in Geant4 [4]. Physical material properties for CdTe were chosen from Strauss (1977) [5]. In the model we used the low energy Livermore physics and enabled Compton scattering, Photoelectric effect as well as gamma modes including fluorescence events. The particle gun was placed $0.5\,\mathrm{mm}$ above the center of the detector. The system's random number generator was used to provide random numbers.

The simulations were controlled by a macro file. A single x-ray photon was used per run. The position information and deposited energy was written to an ASCII file. In order to generate 500 events, Geant4 was started by a Python script that copied and renamed the output to a sub-folder. Only those charges that were in a volume of $220\,\mu\mathrm{m} \times 55\,\mu\mathrm{m} \times 1{\times}10^4\,\mu\mathrm{m}$ were selected for further simulation in the finite element model. These files were further processed in a second Python script where coordinates were transformed to the Medici coordinate system. The deposited energies were converted into charge pairs using a production value of $4.43\,\mathrm{eV}$ and the charge in µC was stored in a separate file per charge cloud.

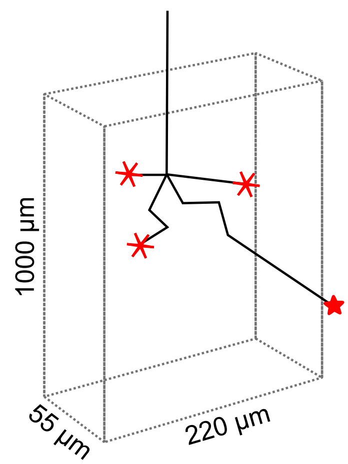

Fig. 1. Event selection for Medici simulations. The dashed line marks the volume simulated in Medici and is located in the center of the detector simulated in Geant4. Events marked with ✻ are placed inside the simulated volume, events marked with ★ are not simulated in Medici.

B. Drift diffusion model with Medici

The charge transport model was implemented using Medici from Synopsys' TCAD suite [6]. The CdTe detector model measured $220\,\mu\mathrm{m}$ in width and $1{\times}10^4\,\mu\mathrm{m}$ in height and had a thickness of $1\,\mu\mathrm{m}$.

Five terminals were placed at the bottom of the device, three of them with the full pixel pitch of $55\,\mu\mathrm{m}$ and those two at the edge measuring half a pixel width. A common cathode was placed on the top and biased with $-300\,\mathrm{V}$. All contacts were defined as Ohmic contacts. To begin with, the finite element model from HgCdTe was chosen and adapted to CdTe. Electrical properties were set for mobility to $75\,\mathrm{cm}^2\,\mathrm{V}^{-1}\,\mathrm{s}^{-1}$ for holes and $1050\,\mathrm{cm}^2\,\mathrm{V}^{-1}\,\mathrm{s}^{-1}$ for electrons. The resistivity was set to about $1{\times}10^8\,\Omega\,\mathrm{cm}$ and the relative dielectric constant adjusted to ϵ = 10.90.

Due to a limitation in Medici, each charge cloud was placed according to its position and simulated in its own simulation file. Charges were collected at the bottom pixels of the device.

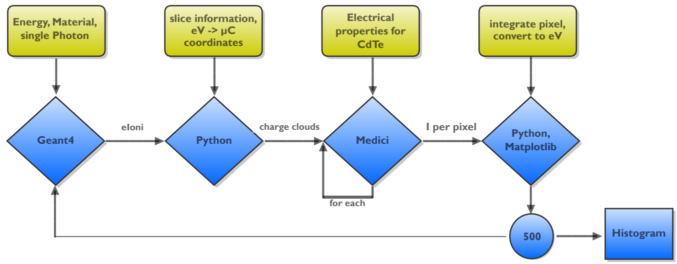

Fig. 2. Workflow for Monte Carlo simulations in Geant4, drift diffusion model with Medici and Python scripts to convert units and coordinates as well as create simulation files automatically.

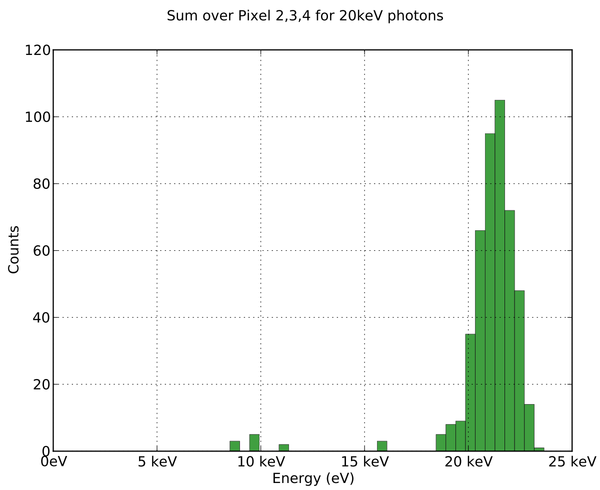

Fig. 3. Sum over charge from three pixels in the center for 20keV X-ray photons. X-ray photons hit the detector in the center of the center pixel.

The measured current was integrated over time. All charges collected from secondary events that originated from the same x-ray photon were kept and set back together.

We generated secondary events from 500 single photons of each of the following photon energies $20\,\mathrm{keV}$, $40\,\mathrm{keV}$. In order to simulate photons hitting between two pixels, we added half a pixel width to the coordinates obtained from the first Geant4 simulation and rerun them in Medici. Each charge cloud took about $3\,\mathrm{min}$ to simulate.

III. Results

We integrated the current from each pixel over time and converted the results with a factor of 4.43 back to eV. Charges collected from secondary events evolved from the same X-ray photon were summed to the center pixel and stored in an array. The histograms were plotted from 500 single photon simulations (see figures 3–6).

IV. Discussion

For both energies the photopeak is clearly visible. The histogram for $40\,\mathrm{keV}$ also shows the escape peaks at lower energies. Figure 3 and 4 as well as 5 and 6 show nearly identical results for photons hitting above the center of a pixel and photons hitting between two pixels due to charge summing.

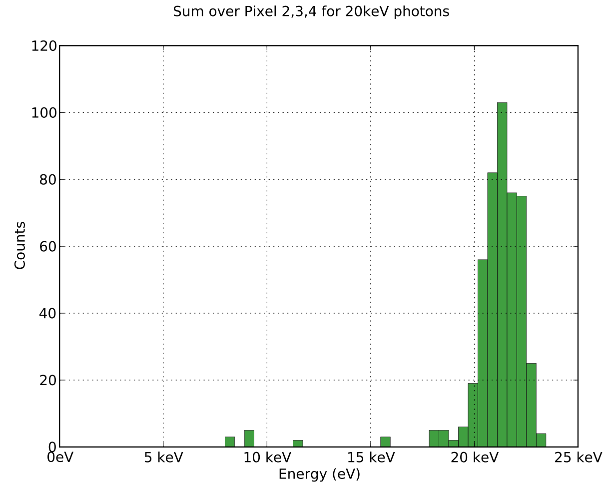

Fig. 4. Sum over charge from three pixels in the center for 20keV X-ray photons. X-ray photons hit the detector between center and neighboring right pixel.

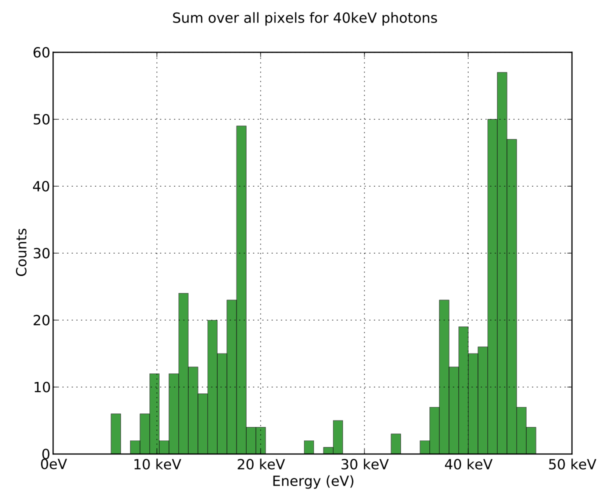

Fig. 5. Sum over charge from three pixels in the center for 40keV X-ray photons. X-ray photons hit the detector in the center of the center pixel.

In the histograms it can be seen that the center of the peak for all energies is slightly shifted to higher energies. This could be due to the mesh geometry in Medici. Charge clouds had to be placed in a square, defined with two sets of x-y coordinate pairs as well as a radius when simulated in Medici. When a charge cloud overlapped two mesh elements a slightly higher charge than deposited is used in the simulation. Refining the mesh could increase the precision but would also increase the running time for each simulation.

V. Conclusion

We successfully combined Monte Carlo simulations with a drift diffusion model in Medici by using Python as scripting language. In this way it is possible to track and simulate drift and diffusion of the charge cloud for each secondary event and study charge sharing between pixels and recreate the deposited

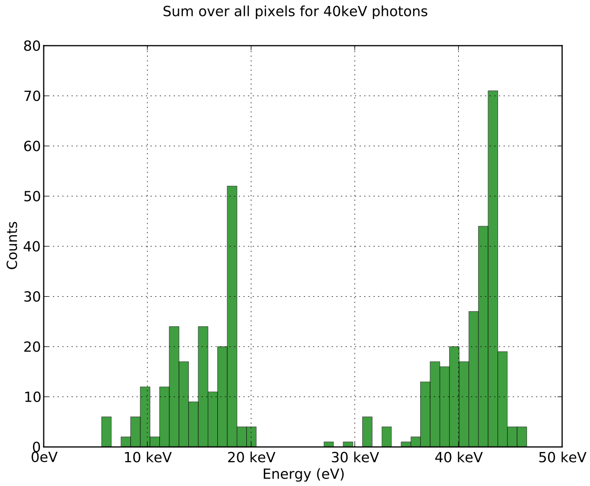

Fig. 6. Sum over charge from three pixels in the center for 40keV X-ray photons. X-ray photons hit the detector between center and neighboring right pixel.

energy. Summing charges from single photons in this idealized model makes it possible to reproduce almost the same results even if the position where the X-ray photon hits the detector is changed.

References

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