









CPPM seminar

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Simulation of hybrid pixel detectors: Validation with XPAD3.2-S/CdTe measurements

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1. Context of the thesis





Detection Technology company:



Medical X-ray imaging Computed tomography Dental imaging Surgical imaging



Security X-ray imaging
Baggage and parcel scan
Cargo and vehicle scan
People scan



Industrial X-ray imaging Food industry

Recycling and sorting Mining industry

- → One axis of the strategy: develop **Spectral Photon Counting solutions**
- → Build an **X-ray chain simulator** as an internal research and development tool for the company

Thesis:

- → **Detection Technology (DT)** leverage the simulation expertise of **imXgam team (CPPM)**
- → Focus on the **simulation of X-ray Photon Counting Spectral Detectors**

Motivation for a simulation of hybrid pixel detectors

- → Early stage of development: detector design optimization
- → Detector operation optimization
- → Create a database for Machine Learning methods
- → Development of correction algorithms
- → Fundamental physics insight of the detector behavior and limitation factors



1. Context of the thesis





Detectors used for the study

| | Amptek: XR-100T-CdTe | CPPM: XPAD3.2-S/CdTe | DT: X-Card ME3 | _ DT : Prototype |
|----------------------------------|--|--|--|--|
| Detectors | PX5 DIGITAL PULSE PROCESSOR Digital Pulse Processor Poster PXR-100-CdTe (1) PXX-RAY DETECTOR | | | |
| Characteristics | Mono-pixel detector 3 mm pitch Cadmium Telluride 1 mm thickness | 2D Matrix 130 µm pitch Cadmium Telluride 750 µm thickness | Linear detector of 128 pixels 800 µm pitch Cadmium Telluride 2 mm thickness Up to 128 bins | 2D Matrix 2x 24x36 pixels 350 – 400 µm pitch Cadmium Zinc Telluride 2 mm thickness Up to 6 bins |
| Impact on simulation development | Reference for understanding physical processes occurring in CdTe | Validation of the simulation on experimental measurements | Generalization of the simulation's model to another detector | Test simulation prediction abilities to anticipate measurement campaign |

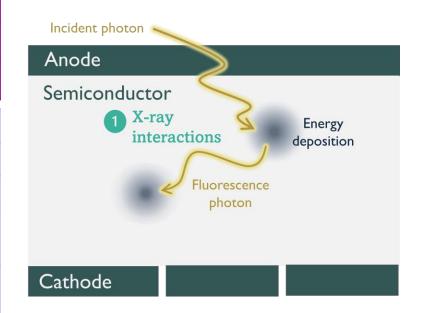
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X-ray interactions Charge carrier dynamics Charge carrier collection

a. X-ray interactions

| Material | Total | Photoelectric | Compton | Rayleigh |
|-----------------|-------|---------------|---------|----------|
| Si (50 mm) | 0.94 | 0.28 | 0.56 | 0.1 |
| CdZnTe (1.6 mm) | 0.94 | 0.87 | 0.04 | 0.04 |
| CdTe (1.6 mm) | 0.94 | 0.89 | 0.03 | 0.02 |

| Material | | Z | K _{α1} [keV] | K _{α2} [keV] | d _{α1} [μm] | d _{α2} [μm] |
|----------|------------|----|-----------------------|-----------------------|----------------------|----------------------|
| Si | | 14 | 1.74 | 1.74 | 11.86 | 11.86 |
| Ge | | 32 | 9.89 | 9.86 | 50.85 | 50.40 |
| GaAs | Ga, 48.20% | 31 | 9.25 | 9.22 | 40.62 | 40.28 |
| uans | As, 51.80% | 33 | 10.54 | 10.50 | 15.62 | 15.47 |
| CdTe | Cd, 46.84% | 48 | 23.17 | 22.98 | 113.20 | 110.75 |
| cure | Te, 53.16% | 52 | 27.47 | 27.20 | 59.32 | 57.85 |



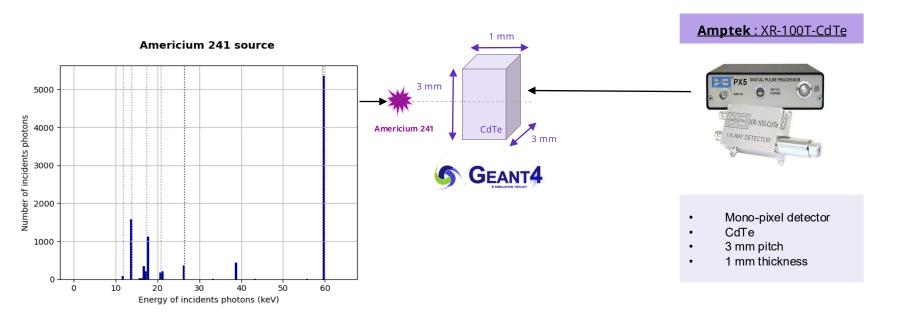
X-ray interactions

Carrier generation

Charge carrier dynamics

Charge carrier collection

- a. X-ray interactions
- Tracking of particles in the sensor, their position and energy loss
- Photoelectric effect, Compton scattering
- CdTe: fluorescence escape photon



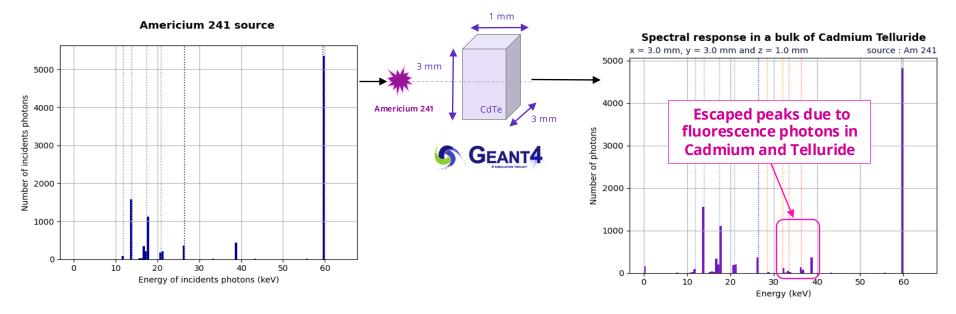
X-ray interactions

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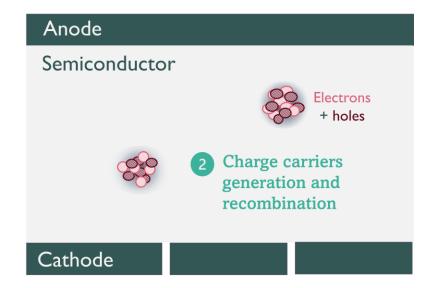
X-ray interactions Carrier generation Charge carrier dynamics Charge carrier collection

- b. Carrier generation and recombination
- Number of e-h generated depends on the material of the sensor
- This number fluctuates (gaussian distribution)

$$\mu=N$$
 $\sigma=\sqrt{(FN)}$ N: Number of charges created

F: Fano factor

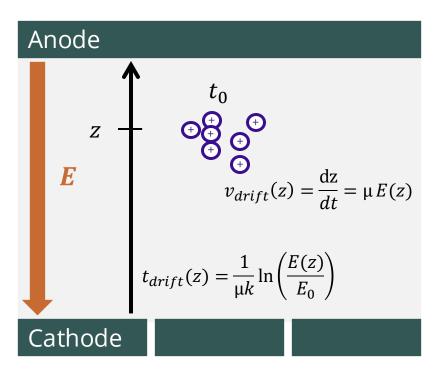
| Material | E _{e/h} | Fano factor | |
|------------------------|-------------------------|-------------|-------|
| Cadmium Telluride | CdTe | 4.43 eV | 0.24 |
| Cadmium-Zinc Telluride | CdZnTe | 4.64 eV | 0.14 |
| Silicon | Si | 3.64 eV | 0.115 |

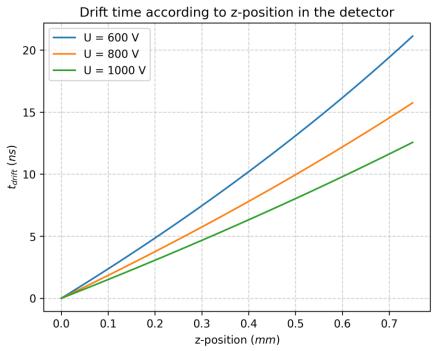


• It is the intrinsic limitation in energy resolution of the detector

X-ray interactions Charge carrier dynamics Charge carrier collection

- c. Charge carrier dynamics
- Charges drift toward the electrodes under the influence of electric field





X-ray interactions Carrier generation Charge carrier dynamics Charge carrier collection

- c. Charge carrier dynamics
- Diffusion and repulsion cause a spontaneous spread of charge carriers
- If size of the electronic cloud increase it may induce **charge sharing**

Charge continuity equation

- Concentration of charge carrier evolution with respect to space and time
- Neglecting generation and recombination at t > 0:

$$\frac{\partial \rho}{\partial t} = D \nabla^2 \rho - \mu \nabla \cdot (\rho \mathbf{E})$$
 Diffusion Electrostatic repulsion

 ρ : Density of charges

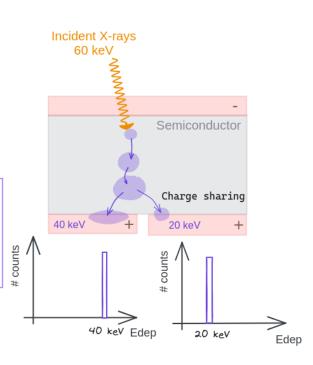
D: Diffusion coefficient

μ: Mobility of charge carriers

E: Electric field induced by charge carriers

Equation solving

 Complex + time consuming in simulation: approximation of the solution using models



X-ray Charge carrier Charge carrier Carrier generation interactions dynamics

- c. Charge carrier dynamics
- The 2 models studied:
 - Repulsion and diffusion are independents E. Gatti et al., NIMA, 253 (1987) 393-399, DOI: 10.1016/0168-9002(87)90522-5.
 - Repulsion and diffusion are **dependents**M.Benoit et al., NIMA, 606 (2009) 508-516, DOI: 10.1016/j.nima.2009.04.019.

Projection on XY electrodes plan $t = t_{drift}$ Charge density Spheric electronic cloud $t = t_1$ Charge density ₹

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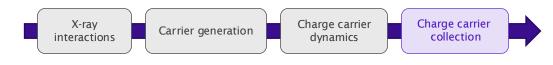
collection

- c. Charge carrier collection
- Electronic noise approximated by a convolution with a gaussian

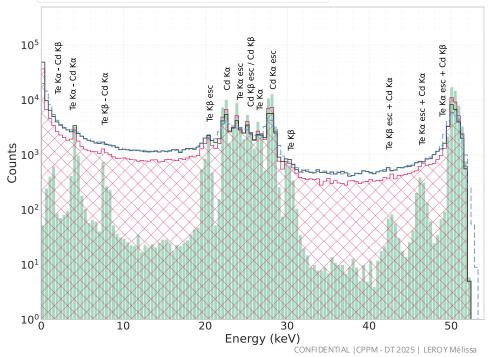
Simulation parameters

| Holes mobility | 100 cm ² /(V.s) | | |
|----------------------|----------------------------|--|--|
| holes lifetime | 2 µs | | |
| Fano factor | 0.24 | | |
| Incident beam energy | 52 keV | | |

- Fluorescence escape peaks are visible on the spectrum
- The full energy peak is shifted due to an incomplete collection of charges
- Activation of diffusion and repulsion increase the size of the electronic cloud and so the charge sharing







3. Experimental validation

c. Comparison of simulation and experimental measurements

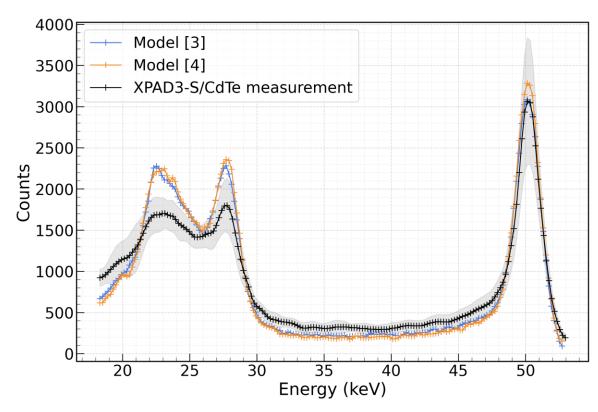




Model [3]: independent

Model [4]: dependent

- Reasonable agreement is observed between the simulations and the mean experimental spectrum
- A higher electronic noise was set to match experimental measurements (close to 170 e - RMS)
- Discrepancies sources can be caused by a non uniform distribution of the threshold steps and some phenomenon are not simulated (pile-up)



4. Conclusion

a. Summary



Goals of the study:

- Development of a simulator capable to reproduce the radiographic chain
- Focus on the simulation of photon counting pixel detector
- Reproduction of the causes of spectral distortion:
 - > Fluorescence escape
 - Charge sharing

Method:

- Development of a simulator integrating charge carrier generation, trapping, dynamics
- Study of 2 charge transport models, essential to reproduce charge sharing
- Processing of XPAD3.2-S/CdTe measurement performed in synchrotron
- Reasonable agreement found between simulation and experimental measurements

Prospects:

- Application of the simulator to other detectors to test its robustness and refine the comparison with experimental data
- Integration of charge induction currently absent from the simulator, to improve the accuracy of the results

Conclusion

b. Next steps





DT: Prototype



- 2D Matrix
- 2x 24x36 pixels
- 350 400 µm pitch
- Cadmium Zinc Telluride
- 2 mm thickness
- Up to 8 bins



- Simulator to be validated against experimental data of CdTe and CZT hybrid pixels prototypes developed by Detection Technology
- ESRF measurement campaign planned from the 10th to 14th December 2025

Thank you

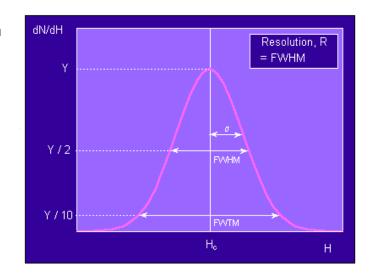


- b. Carrier generation and recombination
- In theory, the variance in the number of charge carriers should follow a stochastic behaviour and therefore a Poisson statistics
- But in really this is a deterministic problem and in real detectors, the observed variance in usually smaller than the one predicted by Poisson statistic.
- Fano factor is the ratio between observed variance and Poisson predicted variance.

$$F = \frac{Observed\,variance\,N}{Poisson\,variance\,(N)}$$

Resolution limit: the statistical limit of energy resolution is:

$$R = 2.35\sqrt(\frac{F}{N})$$



X-ray interactions Carrier generation and recombination

Charge carrier dynamics

Charge carrier collection

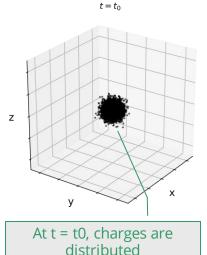
c. Charge carriers dynamics

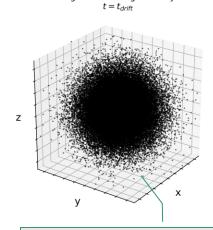
Model 2: Coupling repulsion and diffusion

$$\frac{\partial \rho}{\partial t} = D\nabla^2 \rho - \mu \nabla \cdot (\rho \mathbf{E})$$
Diffusion Electrostatic repulsion

$$\frac{d\sigma^{2}(t)}{dt} = 2\left(D + \frac{\mu N q_{e}}{24\pi^{3/2}\epsilon_{0}\epsilon_{r}\sigma(t)}\right) = 2D_{eff}$$

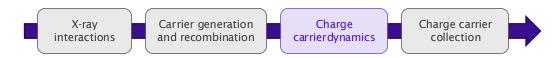
$$D_{eff}$$



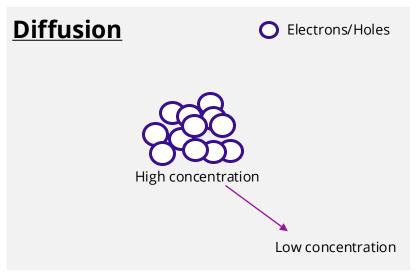


3D gaussian charge density

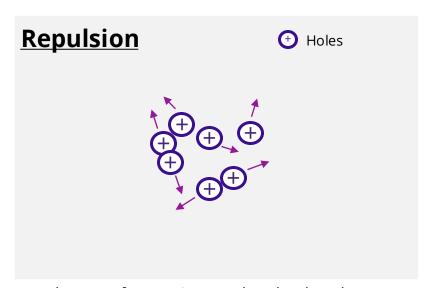
Charges density follows
3D gaussian distribution



- c. Charge carrier dynamics
- Diffusion and repulsion cause a spontaneous spread of charge carriers



An inhomogeneous distribution induce a spontaneous Brownian motion



Charges of same sign repel each other due to electrostatic forces

X-ray interactions Carrier generation and recombination

Charge carrier dynamics Charge carrier collection

c. Charge carriers dynamics

Model 1: Decoupling repulsion and diffusion

$$\frac{\partial \rho}{\partial t} = D\nabla^2 \rho - \mu \nabla \cdot (\rho \mathbf{E})$$
Diffusion Electrostatic repulsion

Diffusion-only equation:

$$\frac{\partial \rho}{\partial t} = D \nabla^2 \rho$$

Repulsion-only equation:

$$\frac{\partial \rho}{\partial t} = -\mu \nabla \cdot (\rho \mathbf{E})$$

X-ray interactions

Carrier generation and recombination

Charge carrier dynamics

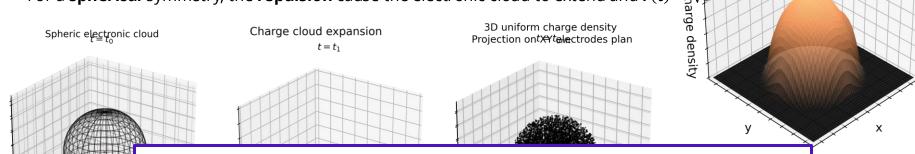
Charge carrier collection

Charge density

Charge carriers dynamics

Model 1: Decoupling repulsion and diffusion

- Repulsion-only equation: $\frac{\partial \rho}{\partial t} = -\mu \nabla \cdot (\rho \mathbf{E})$
- For a **spherical** symmetry, the **repulsion** cause the electronic cloud to extend and $r(t) \ll \sqrt[3]{p}$



Does not stand for energy deposition higher than 10 keV

At t = t₀, charges are concentered in a point

Charges density follows a uniform distribution

$$r(t_{drift}) = \sqrt[3]{\frac{3\mu Nq_e t_{drift}}{4\pi\varepsilon_0\varepsilon_r}}$$

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Z

X-ray interactions Carrier generation and recombination

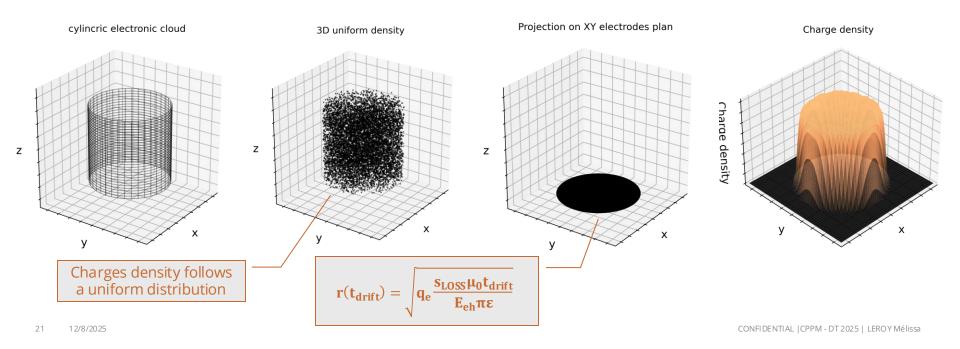
Charge carrier dynamics

Charge carrier collection

c. Charge carriers dynamics

Model 1: Decoupling repulsion and diffusion

• For a **cylindric** symmetry, the **repulsion** cause the electronic cloud to extend and $r(t) \propto \sqrt[2]{t}$



3. Experimental validation

b. Experimental measurements processing



- Calibration for each pixels
- Average over 536 pixels

