GDR, Mi2b

Le 09.10.2024

Simulation of X-ray Photon Counting Spectral Detector

Mélissa LEROY

Plan

1. Context of the thesis
2. Project's progress
3. Conclusion and prospects

1. Context of the thesis

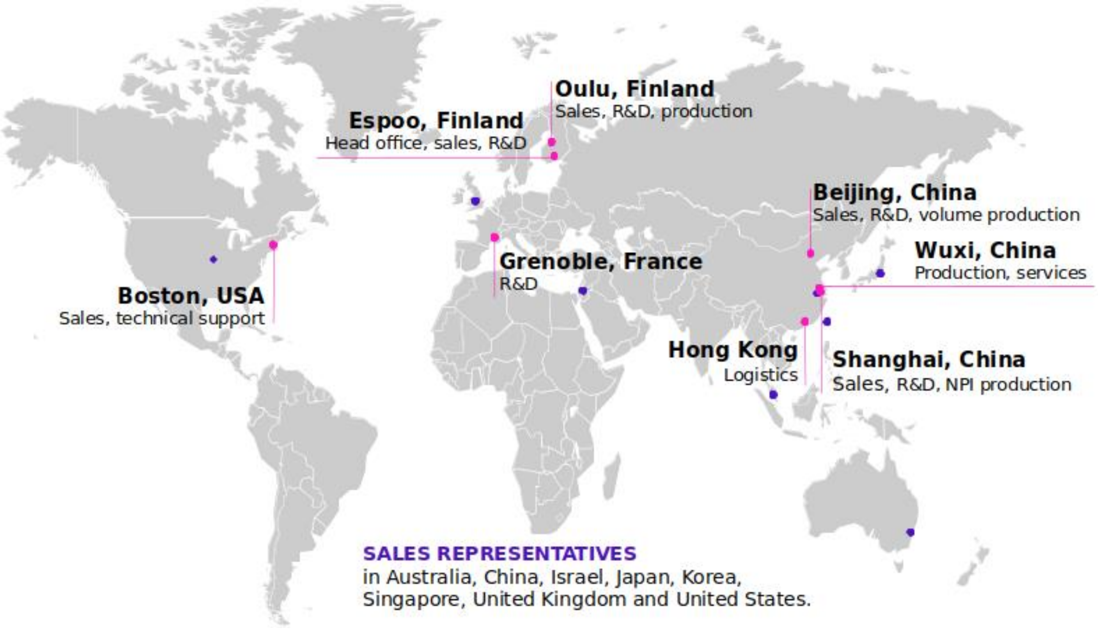
- CIFRE thesis in partnership with the company **Detection Technology (DT)**
- Development of **X-ray detection solutions**
- Applications :

Medical X-ray imaging
Computed tomography
Dental imaging
Surgical imaging

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

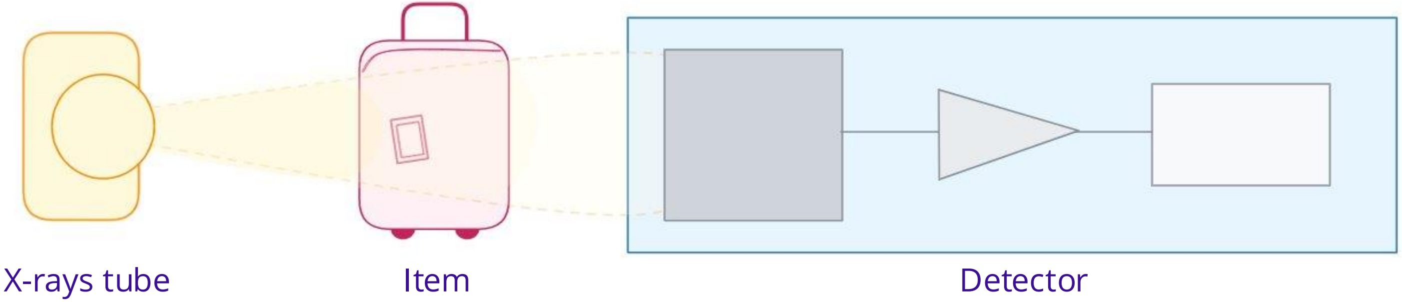
Industrial X-ray imaging
Food industry
Recycling and sorting
Mining industry

- **470 employees** in the world
- **104 M€ net sales** in 2023



1. Context of the thesis

- **Global strategy of the company:**
  → Develop Photon Counting Detectors and associated technology solutions
  → Build an X-ray chain simulator as an internal research and development tool for the company

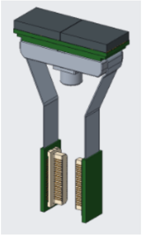
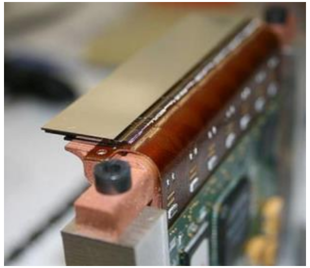


- **Stakes:**
  → Simulate new detectors
  → Evaluate the interest of a detector compare to another for a specific application
  → Create a database for Machine Learning applications

- **Thesis:**
  → Focus on the simulation of X-ray **Photon Counting** Spectral **Detector**

1. Context of the thesis

- **Reproducing technologies…**

	Amptek : XR-100T-CdTe	**DT** : X-Card ME3	**DT** : Prototype	**CPPM** : XPAD3-Si
Detectors				
Characteristics	• Mono-pixel detector • 3 mm pitch • Cadmium Telluride • 1 mm 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 8 bins	• 2D Matrix • 130 µm pitch • Silicon • 500 µm thickness

1. Context of the thesis

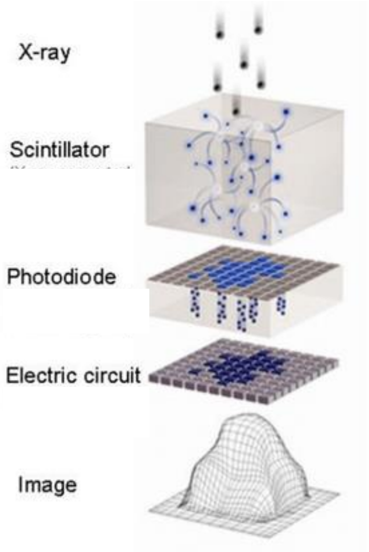
- … and validate simulator's results with experimental results !

From fundamental research to industrial application

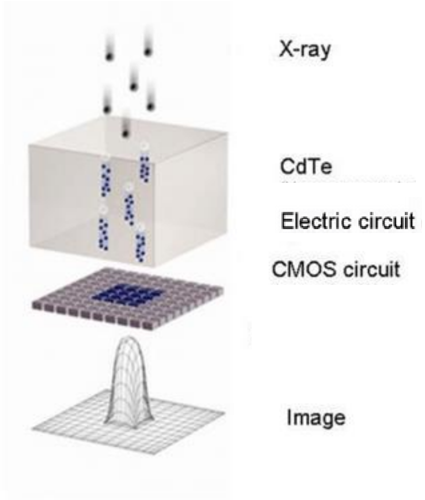
1. Context of the thesis

- **Indirect conversion VS direct conversion**

Indirect conversion



Direct conversion



Indirect conversion:

⊕
- Cheap for customer

⊖
- Electronic noise limitation

Direct conversion:

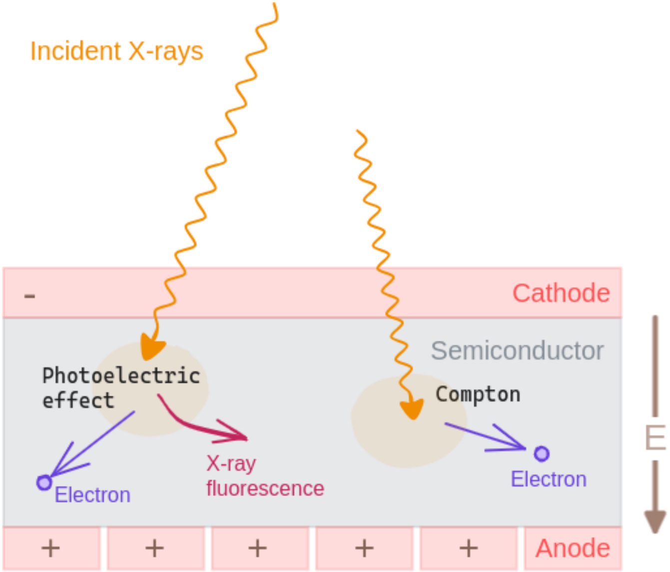
⊕
- Better spatial resolution
- Reduction of the noise
- Better contrast

⊖
- Expensive for the customer

1. Context of the thesis

- **Detection with semi-conductor**

→ X-rays (low energy photons < 250 keV) interact with semiconductor of high atomic number (Z_{Cd} = 48 et Z_{Te} = 52) through photoelectric and Compton effect.

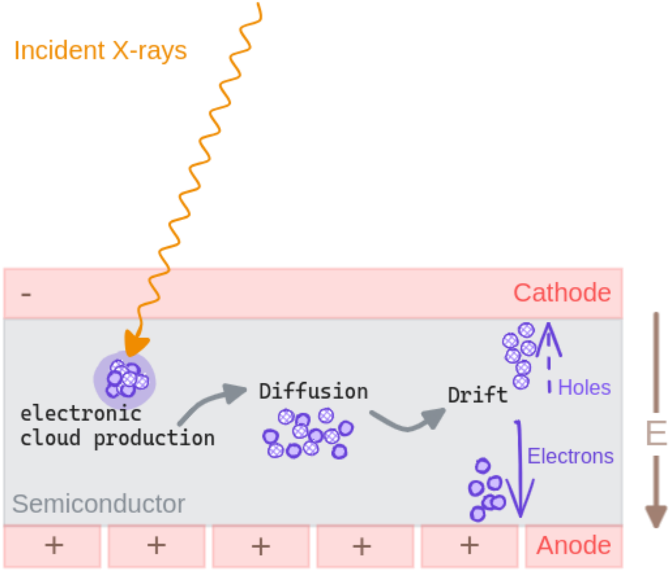


1. Context of the thesis

- **Detection with semi-conductor**

→ X-rays (low energy photons < 250 keV) interact with semiconductor of high atomic number (Z_{Cd} = 48 et Z_{Te} = 52) through photoelectric and Compton effect.

→ The energy deposited in the semiconductor creates electron – holes pairs which numbers depends on the crystal.



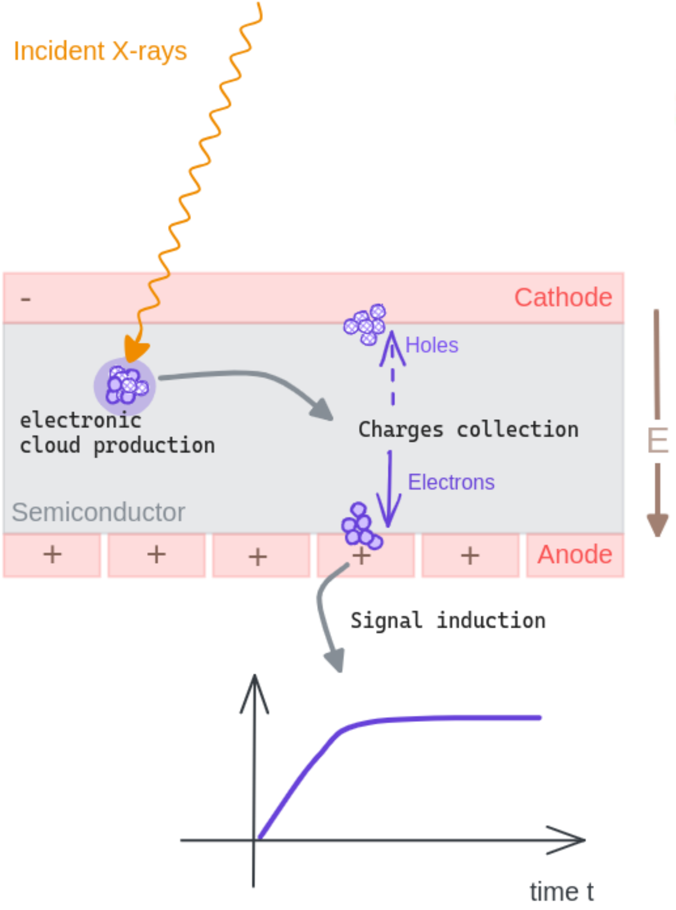
1. Context of the thesis

- **Detection with semi-conductor**

→ X-rays (low energy photons < 250 keV) interact with semiconductor of high atomic number (Z_{Cd} = 48 et Z_{Te} = 52) through photoelectric and Compton effect.

→ The energy deposited in the semiconductor creates electron – holes pairs which numbers depends on the crystal.

→ Charges are separated by an electric field and collected by the electrodes
→ The movement of charges induced a signal on the electrodes
→ This signal is proportional to the energy of incident photons



2. Project's progress

- **Simulation pipeline**

Initial information

- Detector geometry
- X-ray source properties

Energy deposition
Geant4 : Tracking of particles in the sensor, their position and energy loss

→ Location in detector, Quantity of energy deposited

Charges creation
Charges generation : conversion of energy loss into deposited charge carriers regarding the pair energy creation and statistical fluctuation

→ Location, number of charges

Charges transport
Applies drift, diffusion and recombination models

→ Location of charge carriers in the detector

Pixelization
Converts individual charges into a set of charges on the pixels

→ Location and number of charges per pixels

Digitizer
Turns collected charges on pixels into signal and adds a noise contribution

Output information

- Energy spectrum from the simulated detector
- Counts in each of several predefined energy bins

GEANT4 A SIMULATION TOOLKIT (Energy deposition)

Custom code in C++ or in Python (Charges creation to Digitizer)

ap² allpix squared (whole pipeline)

2. Project's progress

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GEANT4 (Energy deposition)

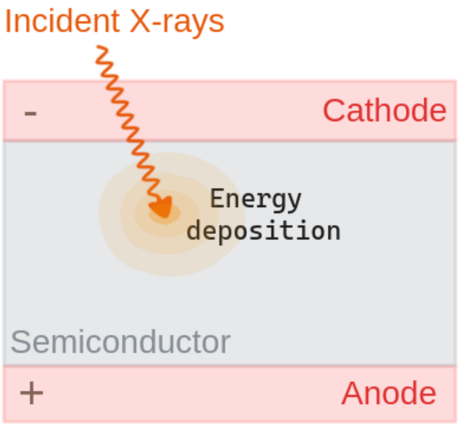
Custom code in C++ or in Python (Charges creation to Digitizer)

What is Allpix Squared?

Allpix Squared is a generic simulation framework for semiconductor tracker and vertex pixel detectors written in modern C++. The goal of the framework is to provide a complete and easy-to-use package for simulating the performance of detectors from incident ionizing radiation until the digitization of hits in the detector chip.

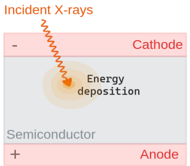
2. Project's progress

- **Simulation pipeline**

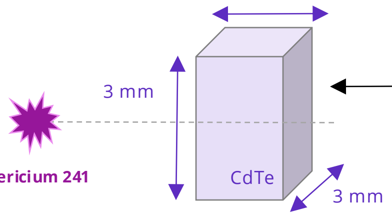


Tracking of particles and their interactions (Photoelectric effect, Compton)

2. Project's progress



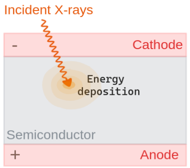
- **Spectrum of an Americium 241 source with Amptek detector**



Amptek : XR-100T-CdTe

- Mono-pixel detector
- CdTe
- 3 mm pitch
- 1 mm thickness

2. Project's progress



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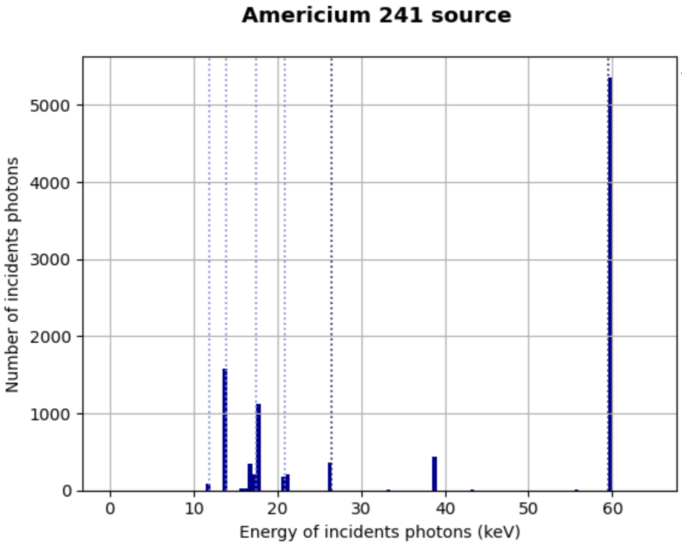
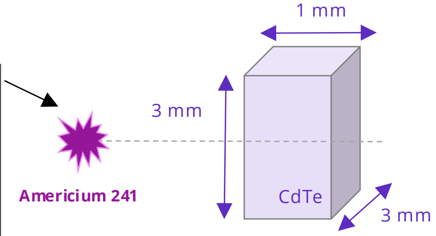
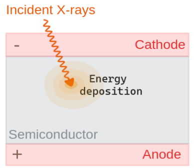




2. Project's progress



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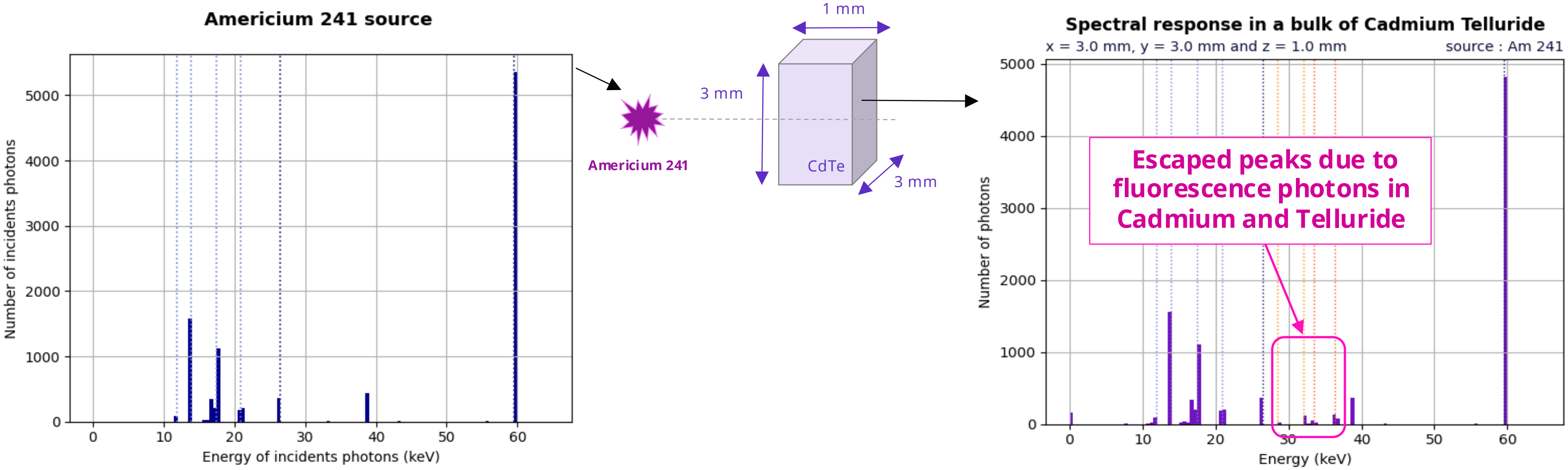
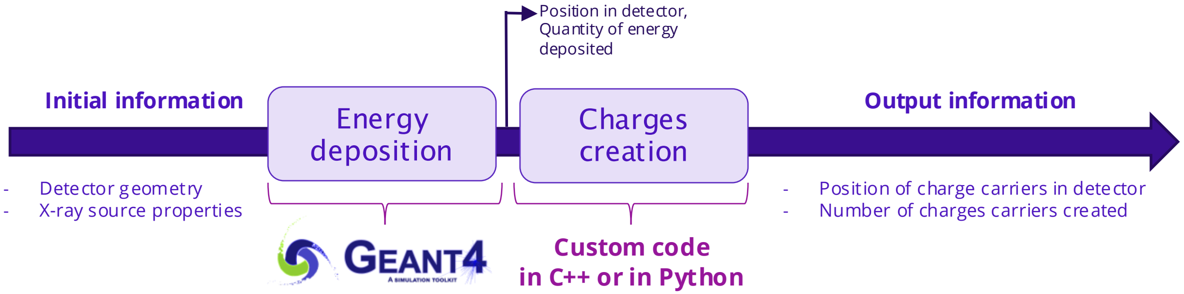


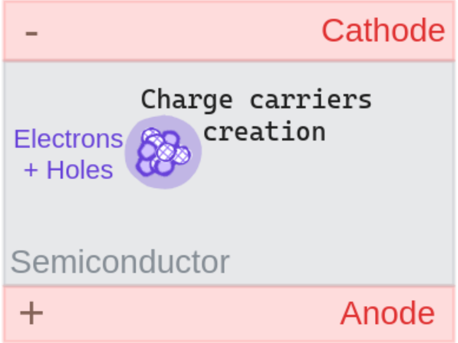
→ Simulation reproduces the Americium 241 source spectra

→ Apparition of new peaks due to escaped **fluorescence photons** after interactions with Cadmium Telluride

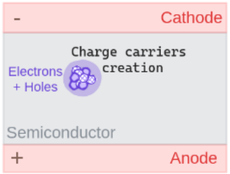
2. Project's progress

- **Simulation pipeline**





2. Project's progress



- **Compute the number of charges created in the sensor**

$$N_{charges} = \frac{E_{deposited}}{E_{e/h}}$$

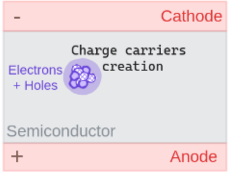
$N_{charges}$: Number of electron-hole pairs created
$E_{deposited}$: Energy deposited in the sensor
$E_{e/h}$: Electron-hole pair creation energy

Material		$E_{e/h}$
Cadmium Telluride	CdTe	4.43 eV
Cadmium-Zinc Telluride	CdZnTe	4.64 eV
Silicon	Si	3.64 eV
Germanium	Ge	2.97 eV
Gallium Arsenide	GaAs	4.2 eV

For a 60 keV in CdTe :
$E_{deposited}$ = 60 keV
$E_{e/h,\ CdTe}$ = 4.43 eV

$N_{charges}$ = 13 544 charges

2. Project's progress



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$E_{deposited}$: Energy deposited in the sensor
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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	0.015
Germanium	Ge	2.97 eV	0.112
Gallium Arsenide	GaAs	4.2 eV	0.14

- **Fluctuations in the number of charge carriers**

→ The process of the electron-hole pair generation could be modeled as a Poisson process.

→ **Fano factor** introduce as an adjustment factor to relate the observed variance to the Poisson predicted variance.

$$F = \frac{\text{Observed variance in } N_{charges}}{\text{Poisson predicted variance}}$$

For a 60 keV in CdTe :
$E_{deposited}$ = 60 keV
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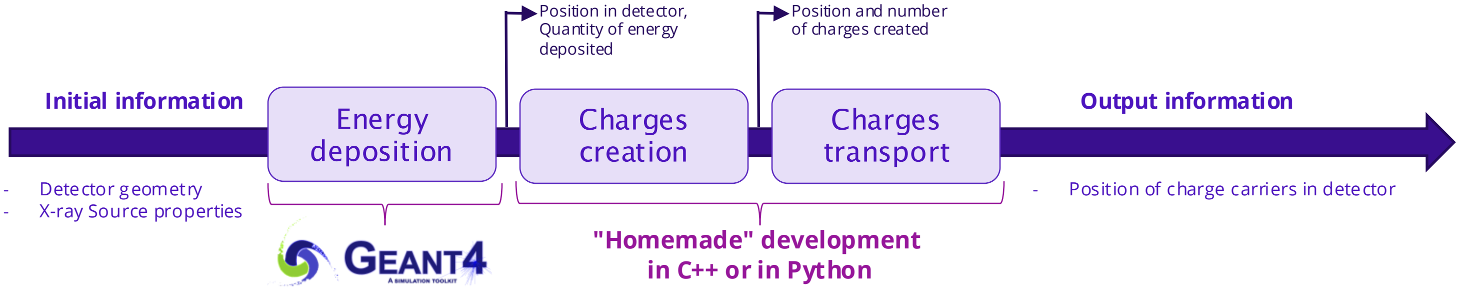
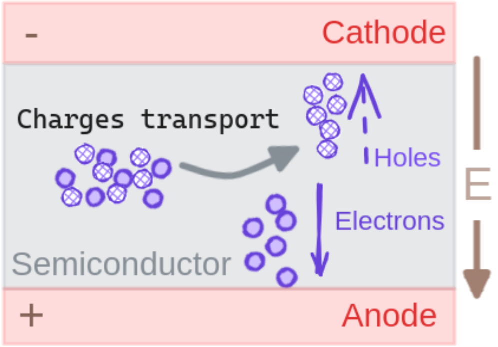
2. Project's progress

- **Simulation pipeline**

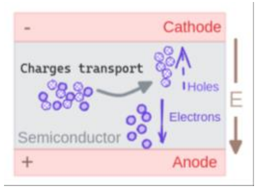


Diffusion: movement due to charge concentration gradient in the semiconductor



Coulomb repulsion: Electric repulsion which pushes away charges which have the same sign

2. Project's progress



- **Continuity equation for electric charges**

→ The dynamics of the electrons is described by the continuity equation:

$$\frac{\partial Q(r,t)}{\partial t} + \underbrace{\mu . E(r,t) \nabla Q(r,t)}_{\text{Electrostatic repulsion}} - \underbrace{D . \Delta Q(r,t)}_{\text{Diffusion}} = 0$$

Q(r,t): Total charge in a sphere of radius r at time t

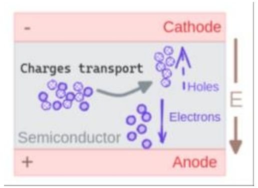
μ: Mobility of charge carriers

E(r,t): Electric field of charge carriers

D: Diffusion constant

- J. Durst, Ph.D. Thesis, Erlangen University, 2008.
- E. Gatti, A. Longoni, P. Rehak, M. Sampietro, Dynamics of electrons in drift detectors, Nucl. Instrum. Methods Phys. Res. A 253 (3) (1987) 393–399.

2. Project's progress



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→ Repulsion-only solution:

$$r_0(t_d) = \sqrt{q \frac{S_{LOSS}}{E_{eh}} \frac{\mu t_d}{\pi \epsilon}}$$

r_0: Cylinder radius (µm)

q: Electronic charge (C)

S_{LOSS}: Stopping power ($MeV.cm^2.g^{-1}$)

E_{eh}: Electron-hole pair creation energy (keV)

µ : Mobility of charge carriers ($cm^2.V^{-1}.s^{-1}$)

t_d : Drift time (s)

ε: Dielectric permittivity ($F.m^{-1}$)

→ Diffusion-only solution:

Diffusion follows Gaussian distribution

$$\sigma(t_d) = \sqrt{2 D t_d}$$

$$D = \frac{\mu . k_B . T}{q}$$

σ: standard deviation of Gaussian distribution

D: Diffusion constant ($cm^2.s^{-1}$)

t_d : Drift time (s)

k_B : Boltzmann constant ($J.K^{-1}$)

T: Temperature (K)

q: Electronic charge (C)

- J. Durst, Ph.D. Thesis, Erlangen University, 2008.
- E. Gatti, A. Longoni, P. Rehak, M. Sampietro, Dynamics of electrons in drift detectors, Nucl. Instrum. Methods Phys. Res. A 253 (3) (1987) 393–399.

2. Project's progress

- **Simulation pipeline**

Initial information
- Detector geometry
- X-ray Source properties

Energy deposition → Position in detector, Quantity of energy deposited

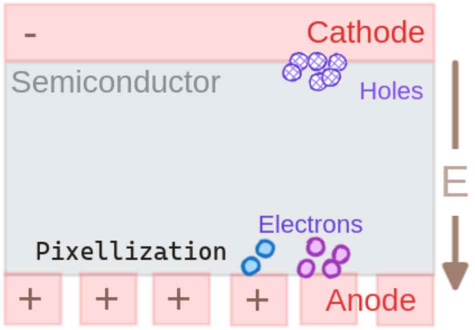
Charges creation → Position and number of charges created

Charges transport → Location of charge carriers in the detector

Pixelization

Output information
- Position and number of charges per pixels

Charge sharing: detection of parts of the initial charge cloud in neighboring pixels. Depends on cloud size (Energy of incident photons & material) and pixel size



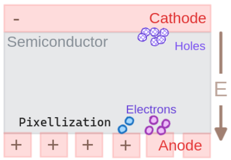
2. Project's progress

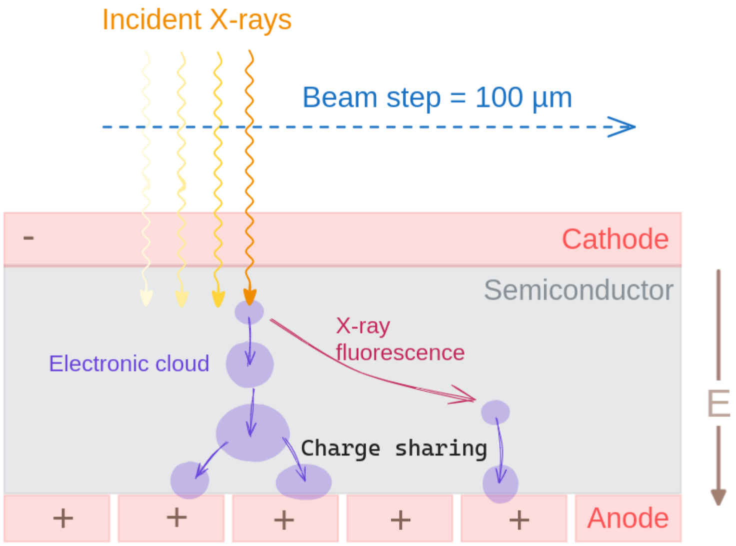
- **ESRF measurement campaign's**
  - → Beamline ID17, 2015
  - → 2 modules of 128 pixels, CdTe (X-Card ME3)

Charge sharing correction study

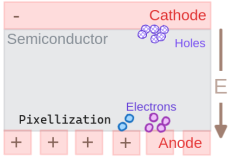
- → Scan of 100 µm step
- → Monochromatic beam of 60 keV
- → Narrow pencil beam (20 µm x 50 µm)
- → 9 positions on two pixels

- **Datas**
  - → 9 Matrices of 256 pixels x 256 channels

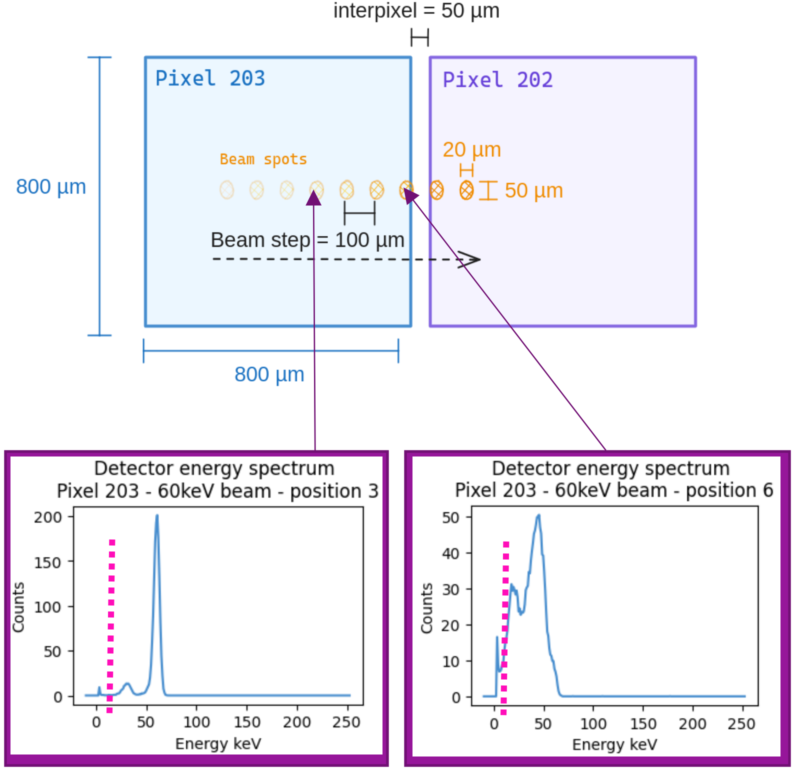




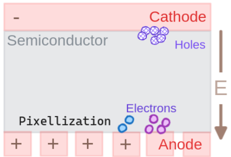
2. Project's progress



- **ESRF measurements analysis**



2. Project's progress



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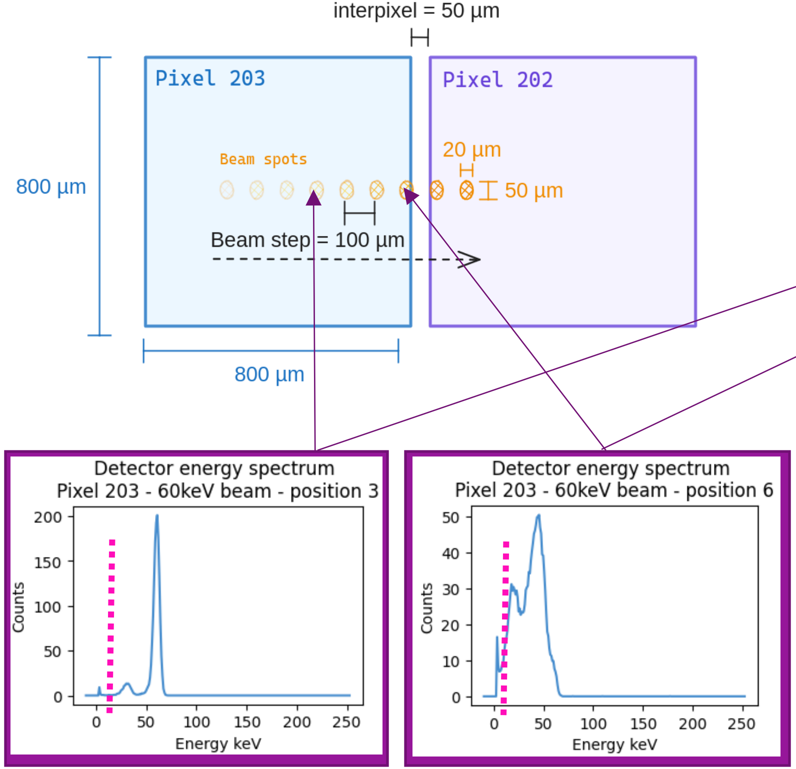
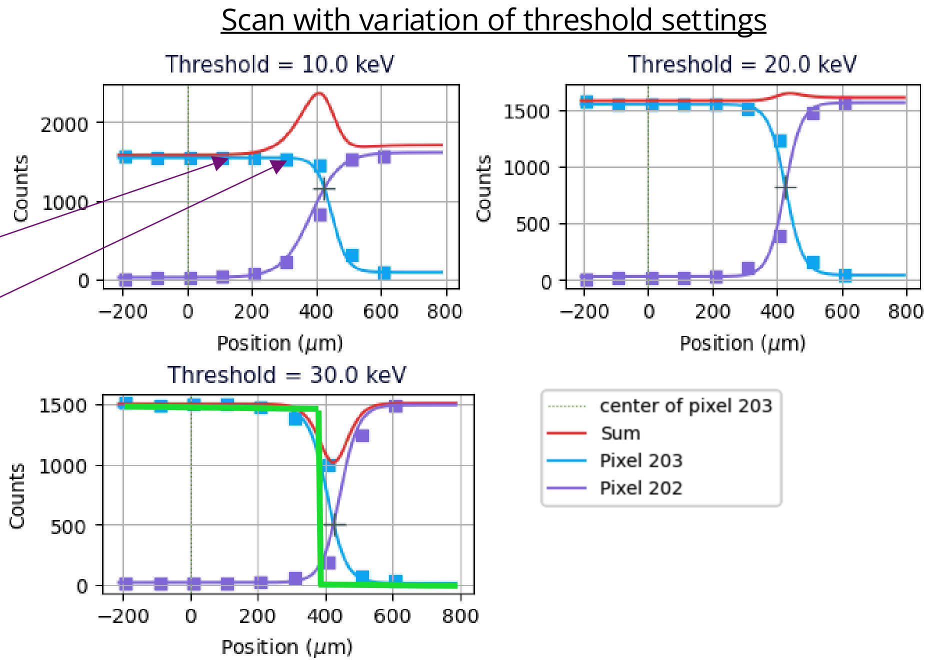




→ A **low** threshold results in **double-counting** in the interpixel area, a **high** threshold **loss of signal**. A threshold of **20 keV** guarantees a **uniform response** of the pixels

2. Project's progress

- **Simulation pipeline**

Initial information

- Detector geometry
- X-ray Source properties

Energy deposition → Position in detector, Quantity of energy deposited

Charges creation → Position and number of charges created

Charges transport → Location of charge carriers in the detector

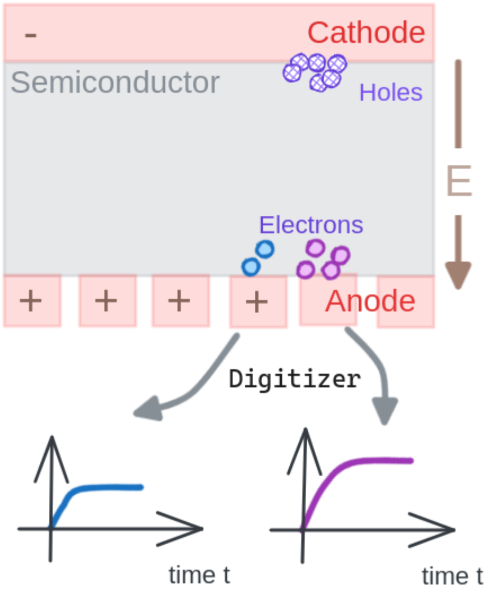
Pixelization → Location and number of charges per pixels

Digitizer

Output information

- Energy spectrum from the simulated detector
- Counts in each of several predefined energy bins

Next component to be developed:
- Signal per pixel
- Electronic noise
- Pile-up effect



3. Conclusion and prospects

- **Conclusion**

→ Simulation pipeline in construction

→ Simulation of physical interactions with Geant4

→ Study of charges dynamics in Silicon with continuity equation

→ Analysis of ESRF measurements of charge sharing study X-Card ME3

- **Prospects**

→ Charges dynamics to study in CdTe

→ Experiment new simulation framework (Allpix squared) to reproduce semiconductor behavior

→ New DT prototype characterization in ESRF

Thank you

Back-up

a. Photoelectric effect

- **Photoelectric effect**

→ An incident photon interact with an electron of the inner shell. It deposits the energy required to eject this electron (binding energy) and gives the rest of its energy to the photoelectron emitted.

→ The photoelectron ejected has an energy equal to the energy of the incident photon minus the binding energy of the electron.

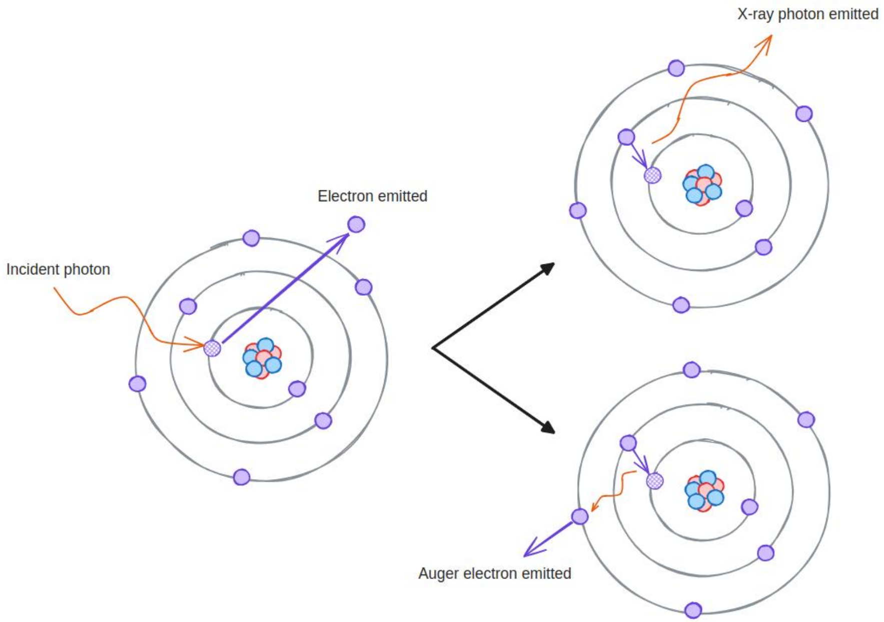
→ This interaction leaves a vacancy in the electron cloud. A relaxation phase ensures that the atom remains stable.

- **Fluorescence**

→ An electron from a higher energy subshell will fill the vacancy. This deexcitation will produces characteristics X-ray photons.

- **Auger cascade**

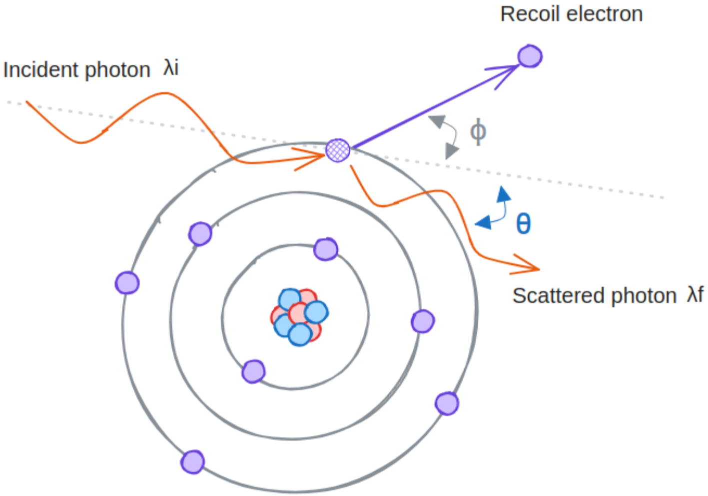
→ The atom will perform a succession of several electronic transitions. It will end in the emission of electrons with low energies (eV).



Back-up

b. Compton effect

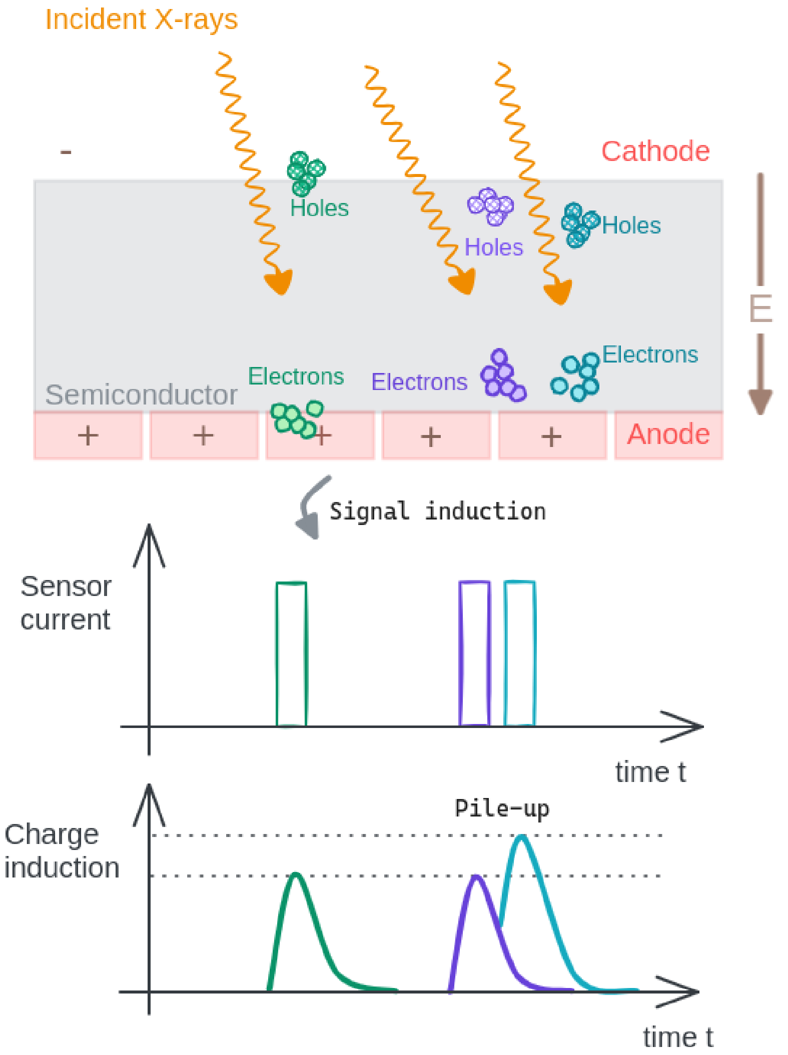
- Qualified as "inelastic scattering"
- The incident photon collides with an electron weekly bounded to the atom. It gives its energy to an electron and is then scattered from its original direction of travel.
- In reality, it is not the same incident photon, it has been absorbed and a new photon, with a lower energy is scattered. The Compton electron is ejected according to a certain angle according to the original photon direction of travel.



Back-up

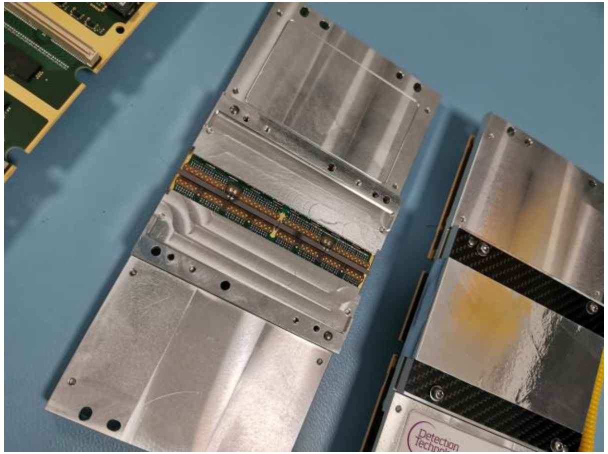
c. Pile-up

- This phenomenon occurs when two photons interact on the same pixel in a very short time. The induced charges can then overlap and cause the convolution of the corresponding signals, which is called a pile-up phenomenon.
- Two events are then treated as one by the processing electronics, which induces an error in the discrimination of their energy.
- The solution to avoid this problem can be to increase the value of the electric field or to reduce the pitch of the anode (and therefore reduce the number of events per pixel) .
- The correct separation of events by electronics is dependent on the minimum processing time, called dead time.
- This phenomenon is not modeled by the detector response function because it is not linear.



Back-up

d. XCard ME



Key characteristics

Parameter	X-CARD ME	X-CARD ME3 XC
Product code	3000027267	3000029815
Sensor type	CdTe semiconductor crystals	
Number of pixels	128	
Intrinsic pixel pitch	0.8 mm	
Crystal thickness	2 mm	
Counting period	0.5 ms to 100 ms / line (step 10 µs)	
Detector binning	1x1 (0.8 mm pitch) or 2x1 (1.6 mm pitch)	
Energy range	20–160 keV	
Number of energy bins	Up to 128	
Linearity	≥ 86% @ 2•106 counts/s/pix	
Saturation	5.0•106 counts/s/pix	> 7.0•106 counts/s/pix
Energy resolution	7.7 KeV @ 60 keV (105 counts/pix/s)	
Adjacent defective pixels	0	
Non adjacent defective pixels	3 (2.3 %)	
Overall uniformity	> -10% < 5%	
Detector element length	128 pixels / 102.3 mm	
Mechanical dimensions	34 mm x 220 mm x 103.5 mm	
Weight	0.70 kg	
Operational voltage and power	48 VDC	
Power consumption per module	28 W	35 W
X-ray tube voltage Vp range	Up to 160 kVp	
EMC compliance	EN 61326-1, EN 61000-4-2, EN 61000-4-3	
RoHS compliance	Yes	
Operational temperature and humidity	0°C to +40°C, 5-95% RH non-condensing	
Storage temperature	-20°C to +60°C	

Back-up

e. Decay chain Americium 241