Spectral Response Simulator of Semiconductor-based X- and Gamma-ray Detectors

M. Bettelli[a], N. Sarzi Amadè[a], B. Garavelli[b], P. Pozzi[b], D. Macera[b], L. Zanotti[b], C. A. Gonano[b], A. Zappettini[a]

***Abstract*— Since CdTe and CZT based detectors are more affected by spectral distortions than semiconductors like Si or Ge, it is crucial to consider the poorer performances of this material when designing a new detector. Contacts have a key-role in detector fabrication. Indeed, not optimized contacts result in low performances, even starting with high quality material. Their engineering in terms of geometry and applied voltage is essential. Due to the wide application fields of semiconductor detectors, the best geometry must be calibrated according to the final purpose of the device. Furthermore, considering that CZT is employed in wide energy range: 1 keV - 10 MeV, several and different interaction processes shall be considered.**

In this framework, a tool able to simulate all the physical process involved in the X- or γ-rays detection, from the radiation absorption mechanisms to the influence of electrodes configuration on the signal generation process, is essential. The capability to predict the detector response and to engineer it before its fabrication is fundamental to realize state-of-art devices.

A novel simulation system based on first principle calculations is presented. It is composed by a Monte Carlo simulator, a Finite Elements Method (FEM) calculator and a numerical computation software with the aim of reproducing the radiation-semiconductor interaction, the weighting/electric fields and the carrier transport/signal induction, respectively. Moreover, the presented tool potentially allows to simulate the entire physical surroundings such as filters, collimators and scattering surfaces. In order to validate the simulator, CZT-based detectors with several contact geometries and device constitutional material have been realized and experimental spectra obtained by these detectors are compared with the computed ones.

***Index Terms*— Semiconductor radiation detector, Numerical simulation, Monte Carlo methods, Spectrum Simulation, Signal Induction**

I. Introduction

Semiconductor-based devices have already replaced classical scintillators in various application fields thanks to the direct conversion of ionizing radiation into an electrical signal. Depending on the final purpose, higher energy and/or spatial resolution and higher efficiency can be easily achieved which makes semiconductors the more advanced technology for radiation detection of x- and γ-photons in the 1 keV - 10 MeV energy range [1] [2] [3]. However, spectra obtained by such devices are not distortion-free. Detectors based on materials like CdTe and CZT, although having several advantages like room temperature functioning and high stopping power, are more affected by spectral distortions related to poorer carrier transport properties and high mean free path of fluorescence photons. A proper design in terms of crystal dimensions, contact geometry and operating conditions can reduce or even suppress the extent of these effects. In this framework, a tool able to simulate all the physical process involved in the X- or γ-rays detection, from the radiation absorption mechanisms to the influence of electrodes configuration on the signal generation process, is essential. The capability to predict the detector response and to engineer it before its fabrication is fundamental to realize state-of-art devices and several methods have already been proposed [4] [5] [6].

M. Bettelli (email: manuele.bettelli@imem.cnr.it), N. Sarzi Amadè (email: nicola.sarziamade@imem.cnr.it) and A. Zappettini (email: andrea.zappettini@imem.cnr.it) are with IMEM CNR, Parma, 43124, Italy.

B. Garavelli (email: bgaravelli@x-next.com), P. Pozzi (email: ppozzi@x-next.com), D. Macera (email: dmacera@x-next.com), L. Zanotti (email: lzanotti@x-next.com) and C. A. Gonano (email: cgonano@x-next.com) are with Xnext s.r.l., Milano, 20127, Italy.

II. Simulator Description

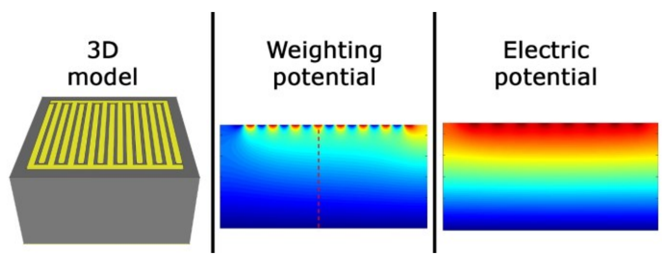

Figure 1. Example of coplanar detector (left) and related weighting (centre) and electric potential (right).

We present a novel simulation system based on first principle calculations which is constituted by three independent blocks. The task of the first part is the simulation of the radiation-matter interaction via a Monte Carlo method. The software allows to design the photon source type (e.g. X-ray tube, a radioisotope), the active material properties (e.g. elemental composition, density, crystal dimensions) and the geometrical configuration of the system (distance from the source and incoming radiation direction). This block returns the interaction positions of each photon by considering the cross section for any possible absorption mechanism (photoelectric effect, Compton scattering, pair production). Potentially, the entire physical surroundings such as filters, collimators and scattering surfaces can be implemented. Thus, an accurate description of secondary radiation can be achieved. Given the crystal dimension, the electrodes patterning and the applied bias, the electric and weighting field can be obtained thanks to the second block which solves the Poisson and Laplace equation through a Finite Elements Method. Any contact geometry can be modelized. For example, in Fig.1 are shown electric and weighting fields for a generic coplanar detector. Finally, the last part combines the results of the two previous blocks and produces the signal induction and the charge collected for each interaction by solving the equations of motion. In Fig.2 carrier trajectories and intensity of induced signals are respectively represented by coloured dots and trail paths.

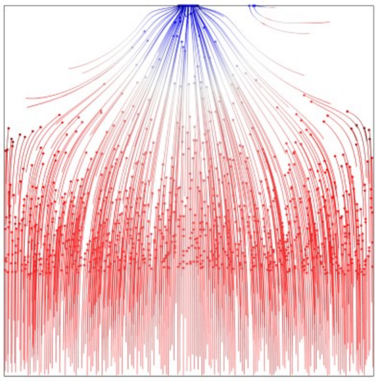

Figure 2. Example of interaction positions and electrons trajectories in a hemispheric detector.

III. RESULTS

In order to validate the simulator, actual CZT-based detectors with extremely different geometries and dimensions have been realized and experimental spectra have been compared with the computed ones. Tests in a wide range of radiation energies (from 25 keV to 660 keV) have been performed in order to underline the capability of reproducing different radiation-matter interaction mechanisms (photoelectric absorption, Compton scattering, CZT fluorescence edges and escape peaks). Comparison between experimental and simulated energy spectra of ^{241}Am nuclear source is shown in Fig3. Simulated spectra are in good agreement with the experimental ones and features like escape peaks and holes trapping are well reproduced. The discrepancies are probably related to secondary radiation which in principle could be eliminated by adding surroundings object which could scatter radiation.

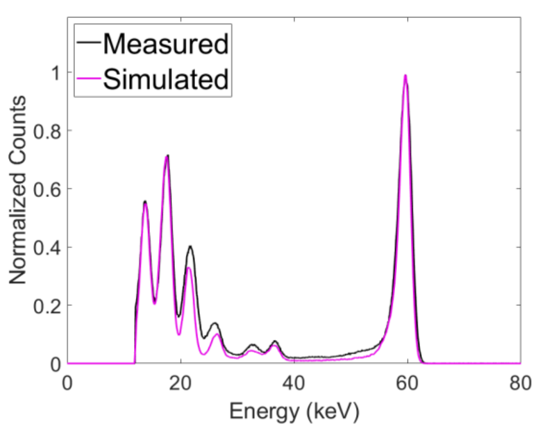

Figure 3. Comparison between experimental and simulated energy spectra of ^{241}Am nuclear source.

IV. CONCLUSIONS

This simulator does not require previous calibration measurements, granting large benefits in terms of time consumption and development costs. Detector design can be accurately optimized before its creation and then realized only once the optimized result has been achieved. Furthermore, the supplementary information provided by this tool, such as electric field, weighting field, and induced current transients, can be very useful to improve the readout electronics or pile-up corrective system based on event pulse shape.

REFERENCES

[1] G. Vedrenne, J.-P. Roques, V. Schonfelder, P. Mandrou, G. G. Lichti, A. Von Kienlin, B. Cordier, S. Schanne, J. Knodlseder, G. Skinner e others, «SPI: The spectrometer aboard INTEGRAL,» *Astronomy \& Astrophysics,* vol. 411, pp. L63--L70, 2003.

[2] S. Del Sordo, L. Abbene, E. Caroli, A. M. Mancini, A. Zappettini e P. Ubertini, «Progress in the development of CdTe and CdZnTe semiconductor radiation detectors for astrophysical and medical applications,» *Sensors,* vol. 9, pp. 3491-3526, 2009.

[3] P. Ubertini, F. Lebrun, G. Di Cocco, A. Bazzano, A. J. Bird, K. Broenstad, A. Goldwurm, G. La Rosa, C. Labanti, P. Laurent e others, «IBIS: The Imager on-board INTEGRAL,» *Astronomy \& Astrophysics,* vol. 411, pp. L131--L139, 2003.

[4] M. Gerlach, M. Krumrey, L. Cibik, P. Müller e G. Ulm, «Comparison of scattering experiments using synchrotron radiation with Monte Carlo simulations using Geant4,» *Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment,* vol. 608, n. 2, pp. 339-343, 2009.

[5] J. Barylak, P. Podgórski, T. Mrozek, A. Barylak, M. Stęślicki, J. Sylwester e D. Ścisłowski, «Geant4 simulations of detector response matrix for Caliste-SO,» *Photonics Applications in Astronomy, Communications, Industry, and High-Energy Physics Experiments 2014,* vol. 9290, p. 929037, 2014.

[6] A. Tomal, J. C. Santos, P. R. Costa, A. H. Lopez Gonzales e M. E. Poletti, «Monte Carlo simulation of the response functions of CdTe detectors to be applied in x-ray spectroscopy,» *Applied Radiation and Isotopes,* vol. 100, pp. 32-37, 2015.