Simulation of Energy-Dispersive X-ray Spectroscopy Systems

Abe Willems[1,2], Sebbe Blokhuizen[1,3], Aron Beekman[1], Thijs Withaar[1,*]

1. Sioux Technologies, Esp 130 Eindhoven, Netherlands
2. Energy Technology, Mechanical Engineering, Eindhoven University of Technology, De Zaale Eindhoven, Netherlands
3. Dept. of Physics, Stockholm University, AlbaNova University Center, SE-106 91 Stockholm, Sweden
* thijs.withaar@sioux.eu

Outline

Full simulation pipeline from electron gun to detector anode

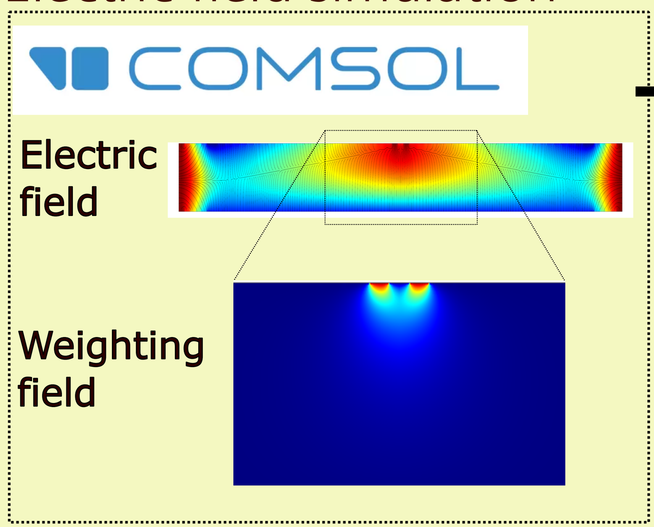
- Geant4 Monte Carlo simulation of electron and photon processes in sample
- Detector electric field modeling with COMSOL
- AllPix^2 simulation of electron-hole transport in detector

Validation against SEM/EDS experiments

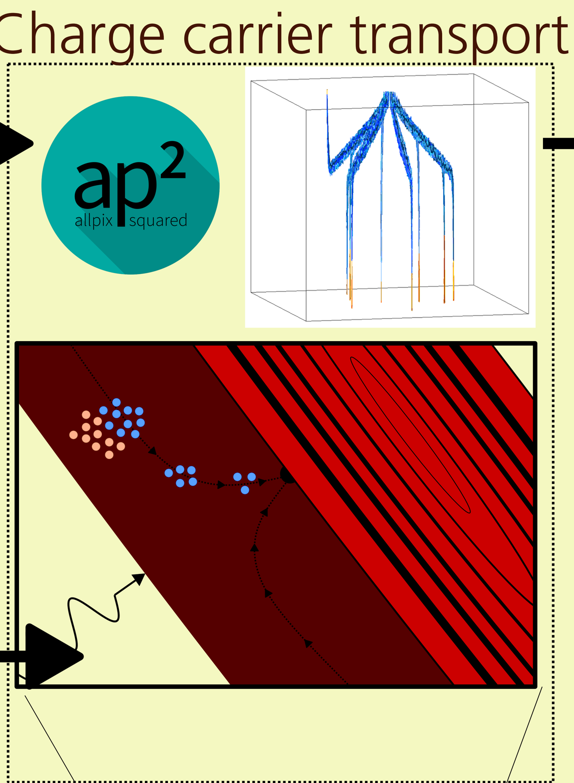
- solve 3D Poisson equation with ring electrodes
- Shockley-Ramo weighting field calculation
- bias voltage parameter sweeps

- SDD faithfully implemented in AllPix^2
- several bugfixes pushed to AllPix^2
  - ROOT writer
  - charge collection deficit
  - GDML geometry import

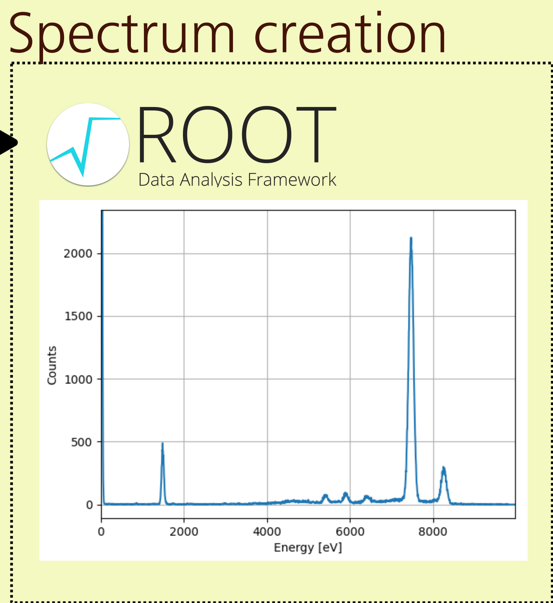
Electric field simulation



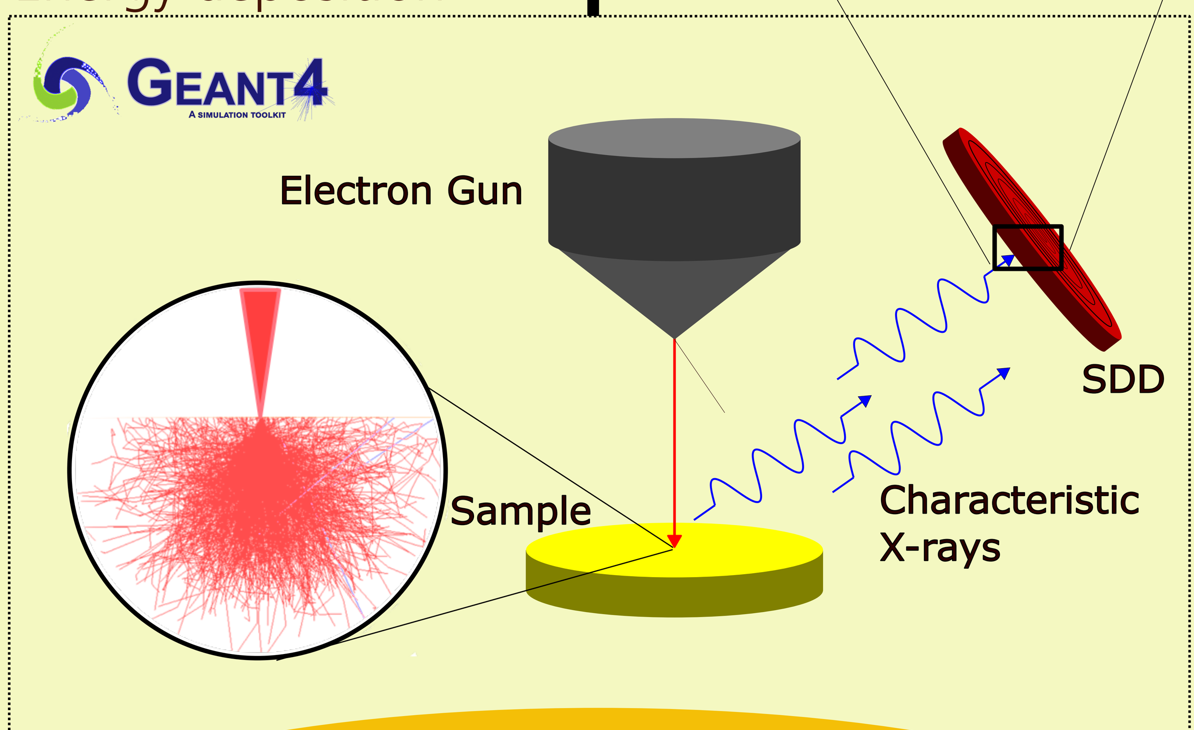
Charge carrier transport



Spectrum creation

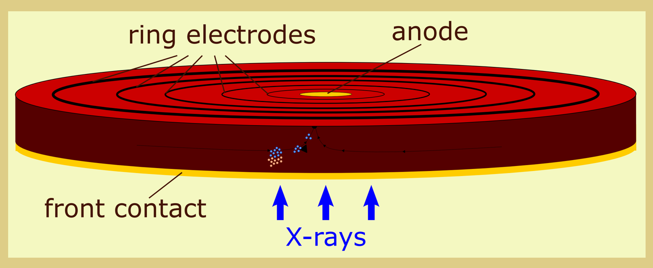


X-ray generation and Energy deposition

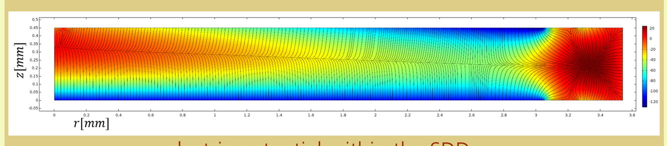


- application in less-studied 100eV – 20keV energy range
- established optimal Geant4 parameters for X-ray generation and energy deposition
- validated low-energy cut-off for relevant electron processes

Silicon drift detectors



Silicon Drift Detectors are X-ray radiation detectors commonly used in XRF and electron microscopy applications.
It is a reversely biased semiconductor where X-rays are converted to electron-hole pairs which are transported to the electrical contacts due to an imposed electric field.



electric potential within the SDD

Despite their apparent simplicity, the details electric field and the charge transport have a large impact on their performance. A slight change in any of the bias voltages can degrade both the energy- and time-resolution of the measurement system.

An important aspect of the charge-transport process is the current induction on the anode. This is governed by the Shockley-Ramo theorem. We use COMSOL or Scikit-FEM to calculate the Shockley-Ramo weighting field directly from the SDD geometry, as an input for AllPix^2.

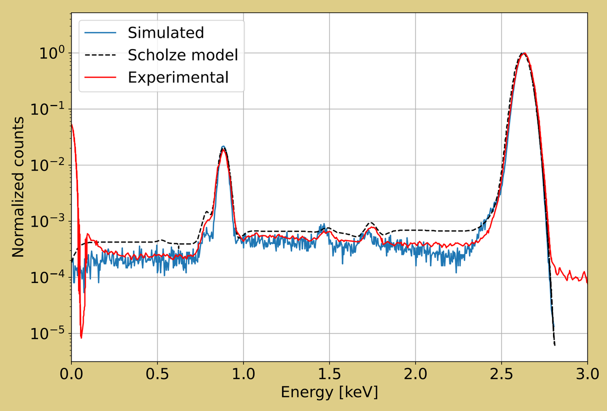
Background

Energy-Dispersive X-ray Spectroscopy (EDS) is an invaluable and ubiquitous elemental quantification and analysis method supplementing Scanning Electron Microscopy (SEM, similar for Transmission EM). Characteristic X-rays from ionization/de-excitaiton events provide detailed information about the elemental composition of the material in focus.

The characteristic peaks in the detected X-ray spectrum are broadened by intrinsic physical processes as well as noise from various parts of the setup. The peak position (X-ray energy) can also shift due to imperfect detection. These spectrum alterations complicate the identification and moreover quantification of the elemental composition.

Here we demonstrate a complete simulation from first principles of the entire SEM/EDS generation and detection process. This can help in the design X-ray measurement systems and ultimately help in updating the semi-empirical φ(ρZ) quantification methods with a model-based method for modern detectors and system geometries.

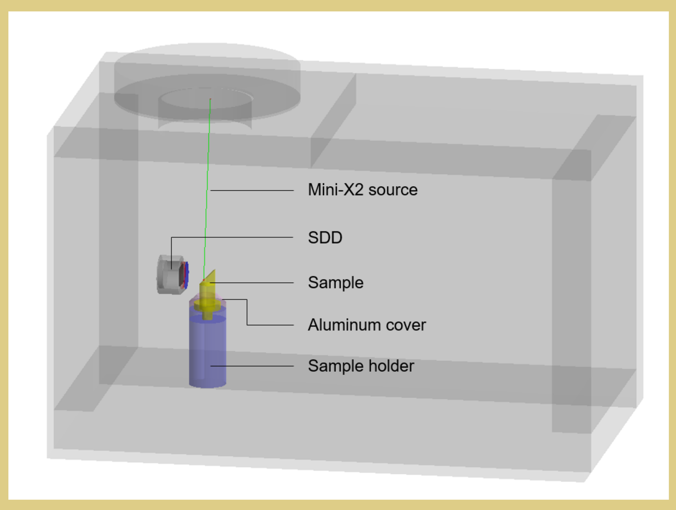
Experimental validation



Response function of an SDD measured and modeled (both from [1]) compared to our simulation.

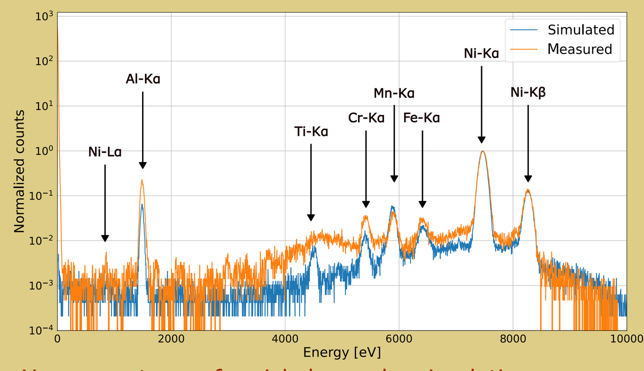
Comparison of the simulation against previous results in literature [1]. The simulation shows a more detailed agreement with the measurements provided in literature than the model given by the authors themselves.
The escape peaks, shelving effects and incomplete charge collection at the left tail of each peak are all visible and close to their measured values.

In order to validate the simulations, a custom setup was built. Here the bias voltages can be controlled, so that incomplete charging effects can be simulated.
The Amptek Mini-X2 X-ray source allows control of both the beam voltage and current, so non-linearities in the electronics due to count rate can be investigated.
Furthermore, with the known geometry, the simulation of system peaks can be validated.

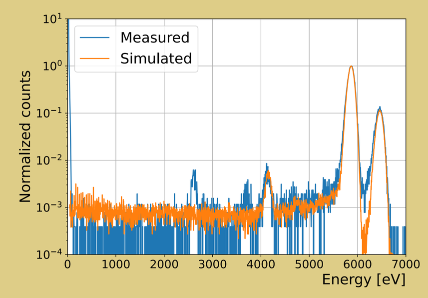


Geometry of the experimental setup.

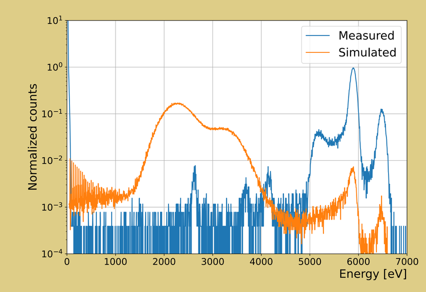
The simulation of the experimental setup also shows good agreement with the measurements. The system peaks of the stainless steel enclosure are close to their expected values, relative to the main peak of the nickel sample. Overall, the shape and intensity of the bremsstrahlung matches well between experiment and simulation, although there is a discrepancy around 5 keV.



X-ray spectrum of a nickel sample, simulation vs. experiment. Both main peaks and contaminations of the stainless steel casing are captured well by the simulation.



Limitations of the simulation start to show up when the bias voltage is off from the optimal value. At the optimal bias voltage (top) almost all the charge generation and transport is correctly tracked, and incomplete charge collection is captured correctly by the simulation.



At deviations from the optimal bias voltage of more than a few percent (bottom) other physics processes preventing charges to reach the anode come into play, which are not taken into account in the simulation.

Experimental and simulated spectra at different SDD bias voltages. Top: optimal value (110V). Bottom: suboptimal value (120V).

Main findings

- With a combination of open source tools, a SEM/EDS system can be simulated in good detail.
  - After a bug-report and -fix, the collected charge in AllPix^2 simulations is correct.
  - Incomplete Charge Collection (ICC) is well captured at optimal bias voltage.
  - System peaks are close to their experimental measurements.
  - The bremsstrahlung is a reasonable match in both shape and intensity.

- Since Geant4 version 11.1.0, the production thresholds can be set correctly for low-energy simulations.
- Geant4 gets main K-peak ratios correct, but underestimates Lλ-peaks.
  ⇨ likely due to limitations of the Atomic De-excitation tables of the Penelope physics model in Geant4.
- The AllPix^2 simulation agrees with semi-empirical model for SDD dead layer [1].
- SciKit-FEM can simulate the electric field of an SDD in a quality comparable to COMSOL.
- The performance of an SDD is *very* sensitive to geometry, doping level and bias voltage.

Future developments

- Entirely replace COMSOL with Scikit FEM to have fully open-source pipeline
- Expand simulation scope to include Scanning Transmission Electron Microscopes
- Improve event bunching and selection to reduce simulation time
- Refine the geometry of the SDD used in the simulation, including the electric field near the PN junction
- Validate the simulation scheme is suitable for other electron and/or photon spectroscopy methods

References

[1] F. Scholze and M. Procop, X-Ray Spectrometry 38 (2009), 312

SIOUX TECHNOLOGIES
TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY
Stockholm University