

Combining COMSOL and Monte Carlo Methods to Simulate SiC Sensors using the Allpix² Framework

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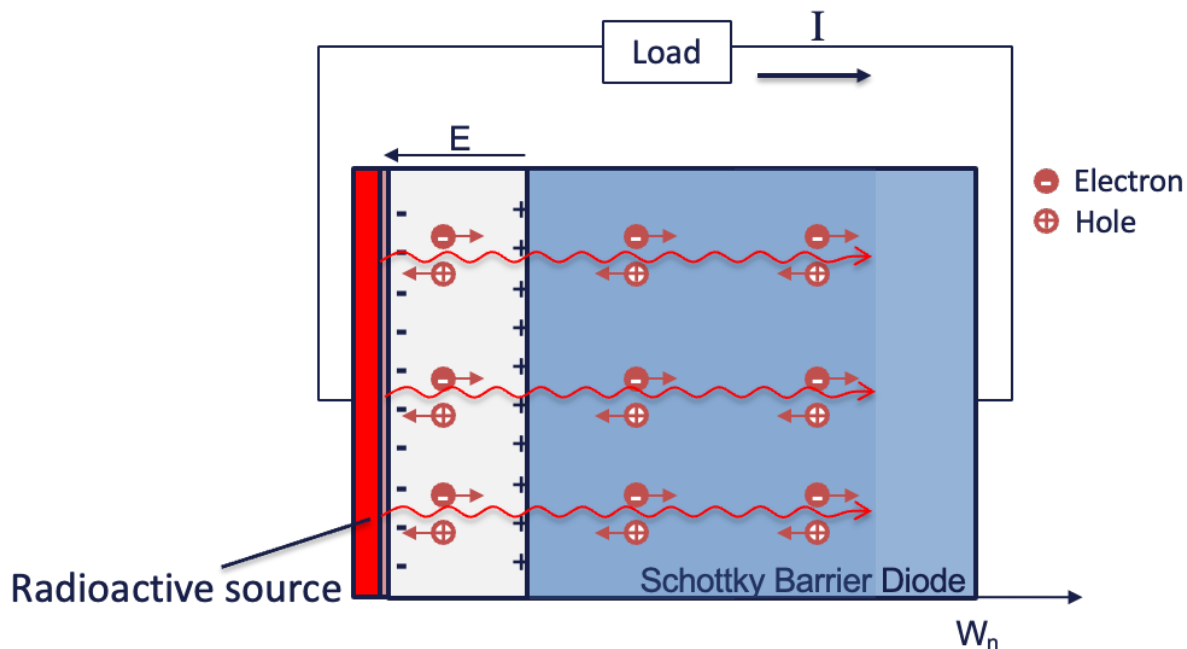
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Introduction

- ❖ Nuclear voltaic batteries based on semiconductor sensors convert the energy from the decay of radioisotopes directly to electricity, as opposed to Radioisotope Thermoelectric Generator (RTG) which is based on the Seebeck effect



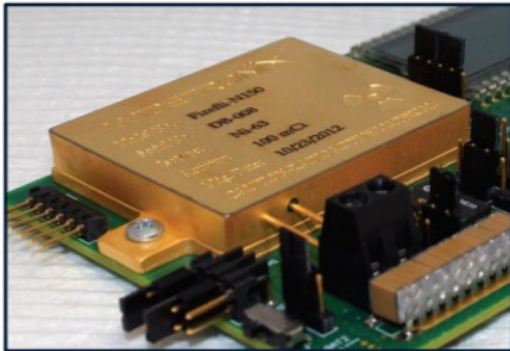
Principle of a nuclear-voltaic battery

Introduction

❖ Major advantages of nuclear voltaic batteries

1) Miniature in size, can be designed from micrometer size to centimeter size

- Can be embedded with the integrated circuits, equipped in the maintenance free sensors and implantable medical devices, etc.



Widetronix, inc

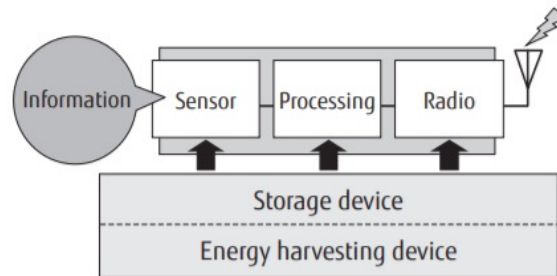
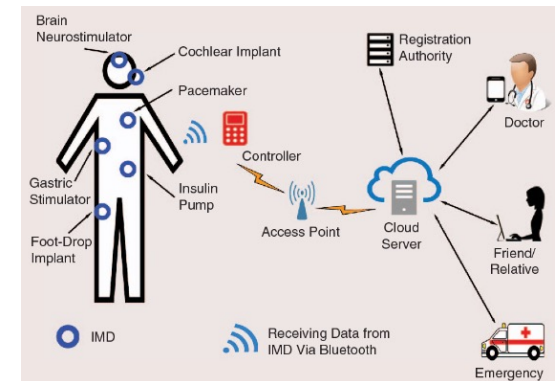


Figure 2
Self-powering wireless sensor module.

Tanaka, et al. Fujitsu Sci. Technol. J, 50, 93-100.

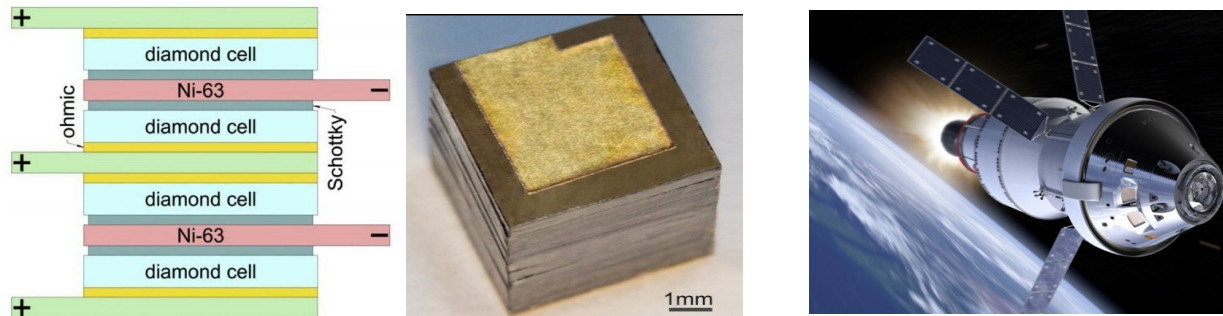
Maintenance free sensors



Implantable medical devices (IMD)

Introduction

- 2) Flexible power output: (nW - μ W)/single battery \rightarrow meet different power demands by by stacking/scaling up



V. Bormashov et al./Diamond and Related Materials

- 3) Stable performance compared to chemical batteries



State-of-the-art and challenges

- Even though the nuclear-voltaic batteries have lots of attractive features, the limitations are also obvious:

- 1) Lowest power conversion efficiency compared to other nuclear battery types

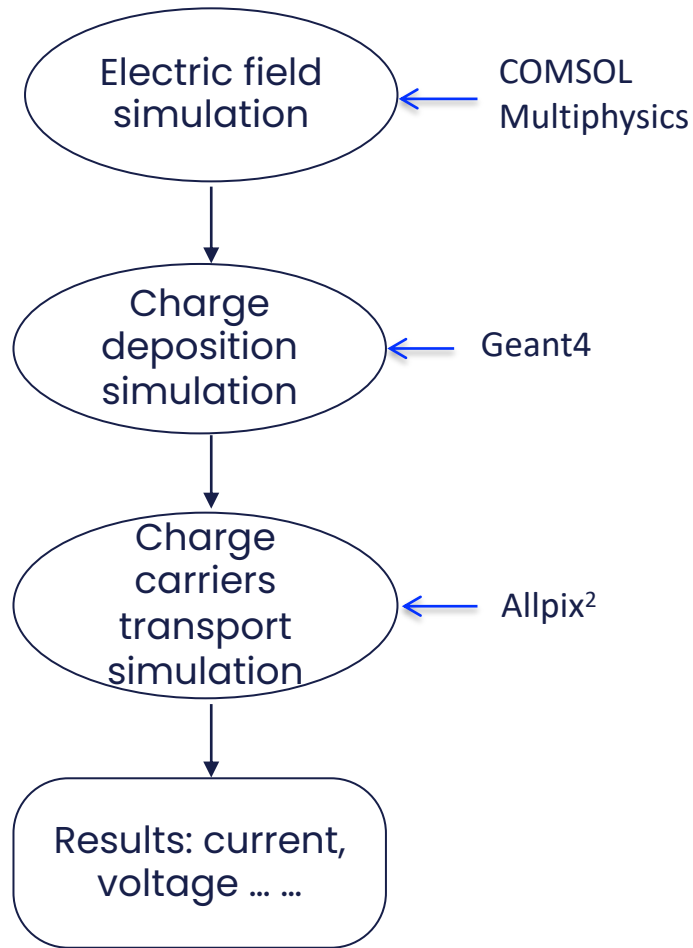
Nuclear-voltaic	RTG	DCNB	RTPV
0.1% ~ 3.6%	10%	15% (theoretically)	31% (theoretically)

- 2) The small output power which is mostly at nanowatt level (highest estimated power density: 25 mW/cm³) can be a disadvantage too
- 3) Radiation damage to the semiconductor material that could reduce the longevity of the battery

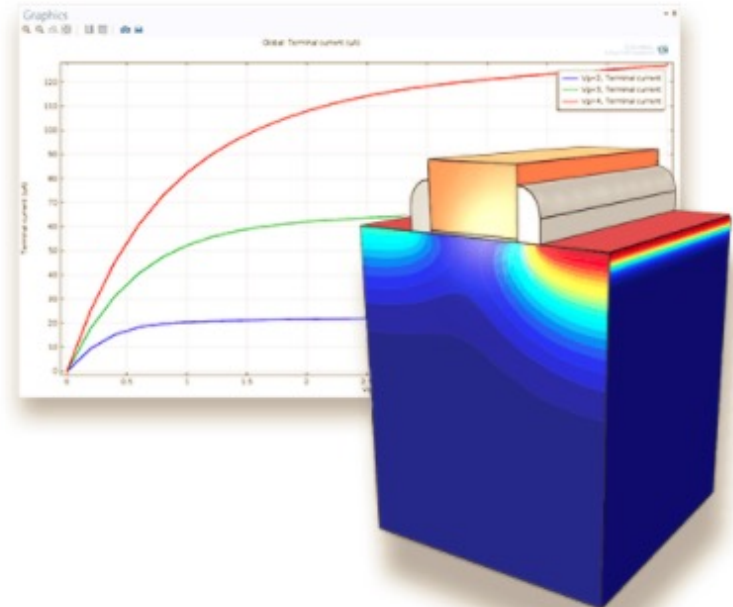
Motivation

- As the nuclear voltaic battery design involves the knowledge of nuclear physics and semiconductor physics, thus accurate simulations are extremely important to optimize the battery design to achieve a higher efficiency/power output
 - Identify appropriate radioactive source
 - Choosing effective source incorporation method
 - Determine the semiconductor sensor's geometric design, structure

Simulation flow of nuclear-voltaic batteries

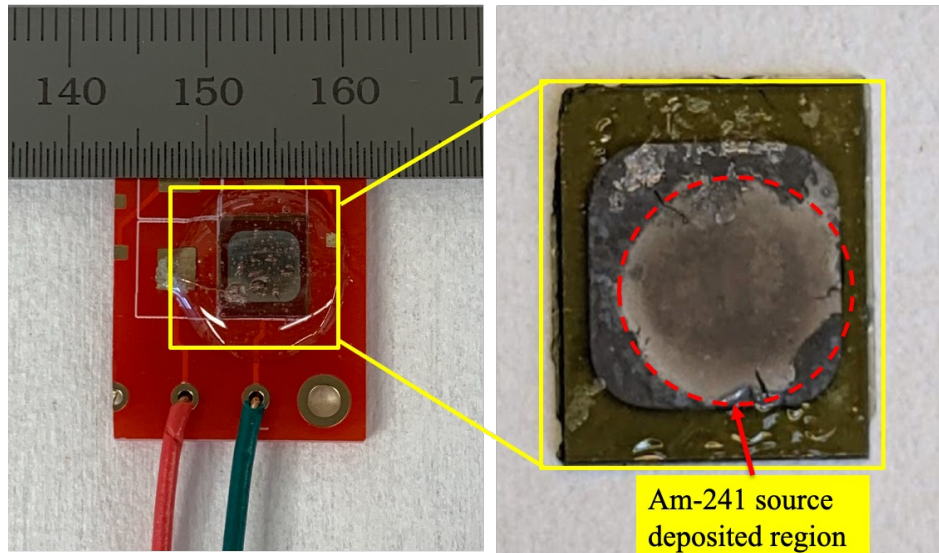


- Semiconductor modeling using the semiconductor module COMSOL Multiphysics:
 - Solves Poisson's equation in conjunction with the continuity equations for the charge carriers
 - Can simulate a wide range of semiconductor devices such as p-n junction, Schottky diodes, MOSFET, MESFET etc.



Simulation of an 4H-SiC Schottky diode sensor with surface electrodeposited Am-241 source

- An in-house fabricated 4H-SiC Schottky diode with surface electrodeposited Am-241 (~ 17 nCi) was simulated and compared to the experimental results
 - This device can be seen as an alpha-voltaic battery but with extremely small source activity

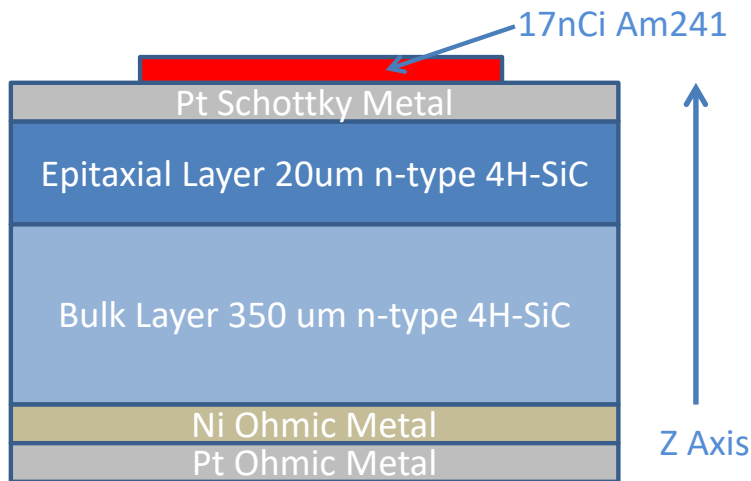


Am-241 electrodeposited 4H-SiC diode sealed in the epoxy (left) and SiC device after electroplating (right)

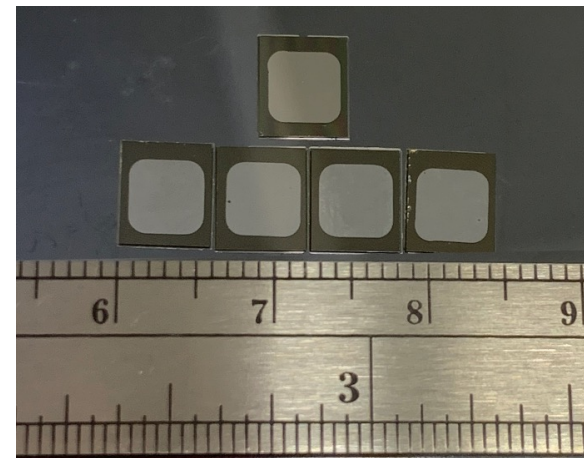
Device structure of the 4H-SiC Schottky diode

❖ 4H-SiC Schottky diode

- 6 mm × 7 mm wafer, 20 μm epi-layer doping concentration: $\sim 2 \times 10^{14} \text{ cm}^{-3}$, 350 μm bulk layer doping concentration: $1 \times 10^{18} \text{ cm}^{-3}$
- 300 nm Pt Schottky contact metal, 4.8 mm x 4.8 mm
- 80 nm/100 nm Ni/Pt Ohmic contact metal



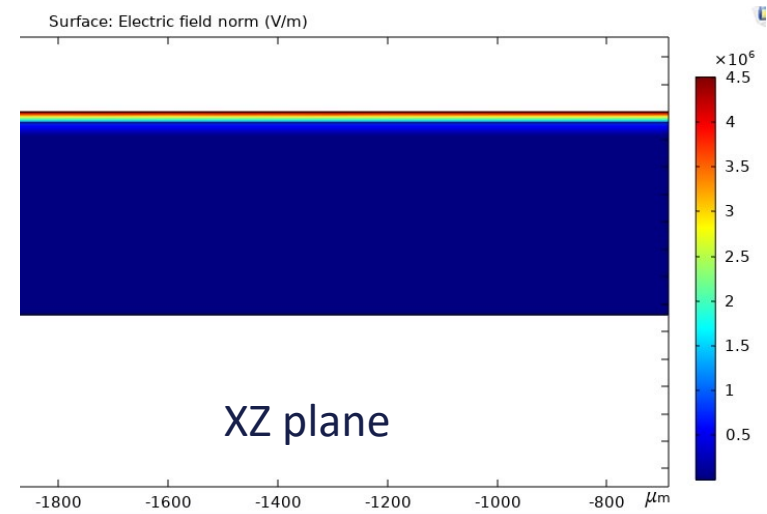
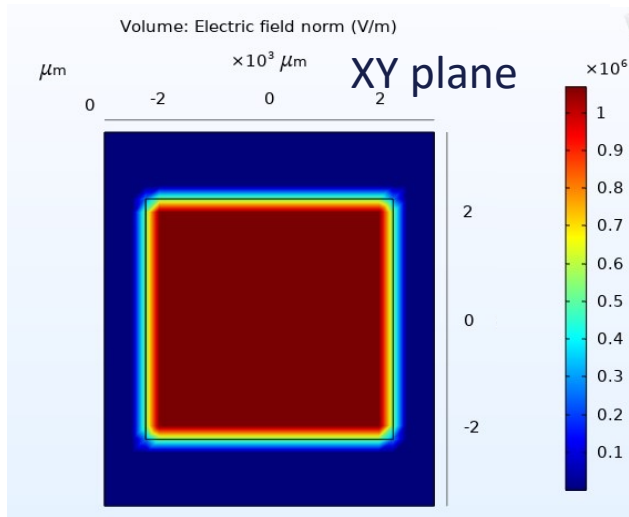
Schematic drawing of the Am-241 electrodeposited SiC Schottky diode



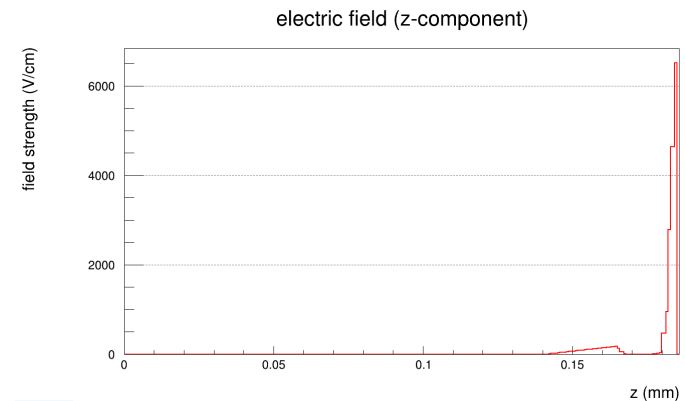
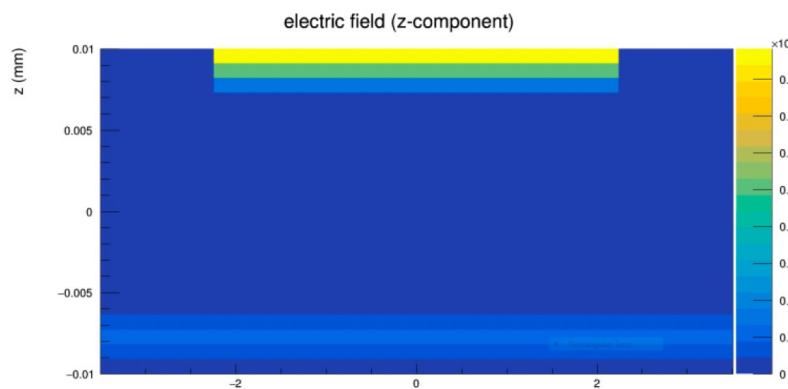
Custom fabricated Pt/SiC Schottky diodes prior to electrodeposition

Electric field simulation of the 4H-SiC Schottky diode

❖ Electrostatic simulation of the SiC Schottky diode



❖ Electric field results were imported to Allpix² using mesh converter



Charge carriers' mobility model

- ✓ The Caughey–Thomas approximation for the low-field carrier mobilities of 4H-SiC was implemented in the Allpix²

$$\mu_{n,p} = \mu_{n,p}^{min} + \frac{\mu_{n,p}^{max} - \mu_{n,p}^{min}}{1 + \left(\frac{N_i}{N_{n,p}^{crit}}\right)^{\delta_{n,p}}}$$

considering the temperature dependence of the parameters, the equation becomes

$$\mu_{n,p} = \mu_{n,p}^{min,0} \left(\frac{T}{300K}\right)^{\alpha_{n,p}} + \frac{\mu_{n,p}^{max,0} \left(\frac{T}{300K}\right)^{\alpha_{n,p}} - \mu_{n,p}^{min,0} \left(\frac{T}{300K}\right)^{\beta_{n,p}}}{1 + \left(\frac{T}{300K}\right)^{\gamma_{n,p}} \left(\frac{N_i}{N_{n,p}^{crit,0}}\right)^{\delta_{n,p}}}$$

Table 1. Caughey–Thomas fit parameters for carrier mobilities in 4H-SiC

Carrier type	$\mu^{min,0}$ cm ² V ⁻¹ s ⁻¹	$\mu^{max,0}$ cm ² V ⁻¹ s ⁻¹	$N^{crit,0}$ cm ⁻³	α	β	γ	δ	Reference
Electrons	40	950	2×10^{17}	-0.5	-2.4	-0.76	0.76	[3]
Holes	15.9	124	1.76×10^{19}	0	-1.8	0.00	0.34	[4]

Charge carriers' mobility model

Perovskite

Project information

Repository

Issues 0

Merge requests 0

CI/CD

Security & Compliance

Deployments

Monitor

Infrastructure

Packages & Registries

Analytics

Wiki

Snippets

Settings

ap²

Allpix²

Generic Pixel Detector Simulation Framework

Allpix² is a generic simulation framework for silicon detectors, written in modern C++. The goal of the Allpix² framework is to provide a comprehensive and easy-to-use package for simulating the performance of silicon detectors from incident ionizing radiation digitization of pixel hits in the detector ASIC.

For more details about the project please have a look at the website at <https://cern.ch/allpix-squared>.

AAT & OSU Collaboration Version

NOTE: This version of Allpix² has been modified as part of a research collaboration between AwareAbility Technologies (AAT) State University (OSU). The baseline for this project was a pull (master) from the cern GitLab repository made on 8/16/2021.

Dependencies

```
src/physics/Mobility.hpp  
289 + class SicRoschke : public MobilityModel {  
290 + public:  
291 + SicRoschke(double temperature, bool doping)  
292 + : electron_mumax(Units::get(950. * std::pow(temperature / 300., -2.4), "cm2/V2s")  
293 + electron_mumin(Units::get(40. * std::pow(temperature / 300., -0.5), "cm2/V2s")  
294 + electron_nref(Units::get(2.0e17 * (temperature / 300.), "/cm/cm/cm")),  
295 + electron_gamma(0.76),  
296 + hole_mumax(Units::get(117. * std::pow(temperature / 300., -2.4), "cm2/V2s")  
297 + hole_mumin(Units::get(33. * std::pow(temperature / 300., -0.5), "cm2/V2s")  
298 + hole_nref(Units::get(1.0e19 * (temperature / 300.), "/cm/cm/cm")),  
299 + hole_gamma(0.5),  
300 + Vmax(Units::get(4.77e7, "cm/s")) {  
301 + if(!doping) {  
302 + throw ModelUnsuitable("No doping profile available");  
303 + }  
304 +  
305 + Vsat_ = Vmax_ / ( 1.0 + ( 0.6 * std::exp(temperature / 600.));  
306 + beta_ = 0.816 + 0.0427 * std::exp((temperature - 327.)/98.4 );  
307 + }  
308 +  
309 + double operator()(const CarrierType& type, double efield_mag, double doping) const {  
310 + if(type == CarrierType::ELECTRON) {  
311 + double mu0 = electron_mumin_ + (( electron_mumax_ - electron_mumin_ )  
312 + / (1.0 + std::pow(std::fabs(doping) /  
313 + electron_nref_,electron_gamma_ ));  
314 + return mu0 / std::pow(( 1. + std::pow( (mu0 * efield_mag)/Vsat_,beta_)),  
315 + ) else {  
316 + double mu0 = hole_mumin_ + (( hole_mumax_ - hole_mumin_ )  
317 + / (1.0 + std::pow(std::fabs(doping) / hole_nref_  
318 +  
319 + return mu0 / std::pow(( 1. + std::pow( (mu0 * efield_mag)/Vsat_,beta_)),  
320 + ) }  
321 + };  
322 +
```

Addition of 4H-SiC mobility model

parent 10574bac master

No related merge requests found

Changes 2

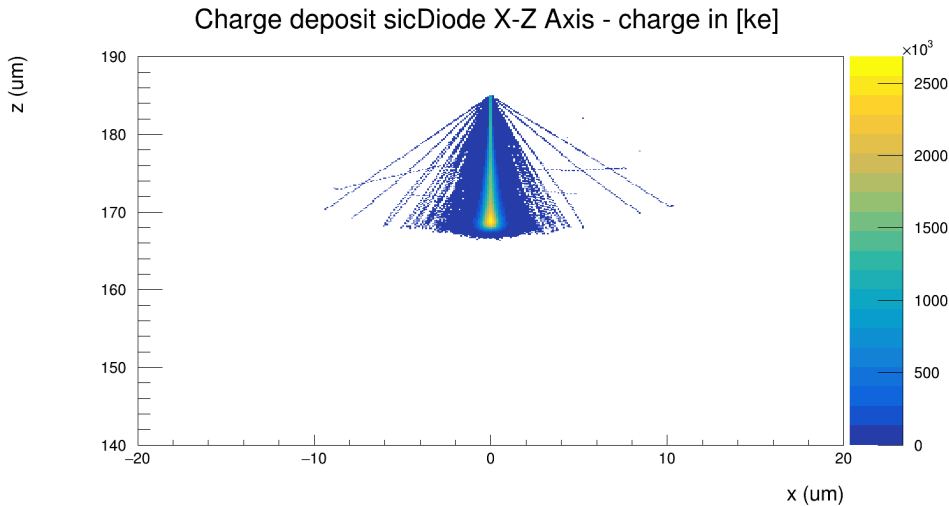
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Hide whitespace changes Inline Side-by-side

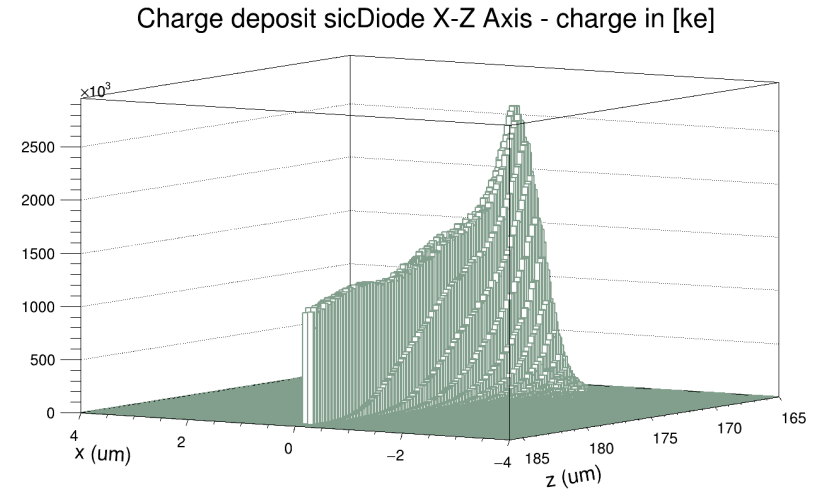
```
src/modules/SicPropagation/SicPropagationModule.cpp  
1 1 /**  
2 2 * @file  
3 3 - * @brief Implementation of perovskite charge propagation module  
4 4 + * @brief Implementation of 4H-SiC charge propagation module  
5 5 * @remarks Based on code the Generic Propagation Module  
6 6 * @copyright Copyright (c) 2021 AwareAbility Technologies LLC.  
7 7 * Also contains : Copyright (c) 2017-2020 CERN and the Allpix Squared authors.  
... ... @@ -70,7 +70,7 @@ SicPropagationModule::SicPropagationModule(Configuration& config,  
70 70 config_setDefault<double>("temperature", 293.15);  
71 71  
72 72 // Models:  
73 73 - config_setDefault<std::string>("mobility_model", "jacoboni");  
74 74 + config_setDefault<std::string>("mobility_model", "sic_roschke");  
75 75 config_setDefault<std::string>("recombination_model", "none");  
76 76  
... ... config_setDefault<bool>("output_linegraphs", false);
```

Simulation results-charge creation in the SiC sensor

✓ Charge deposition results



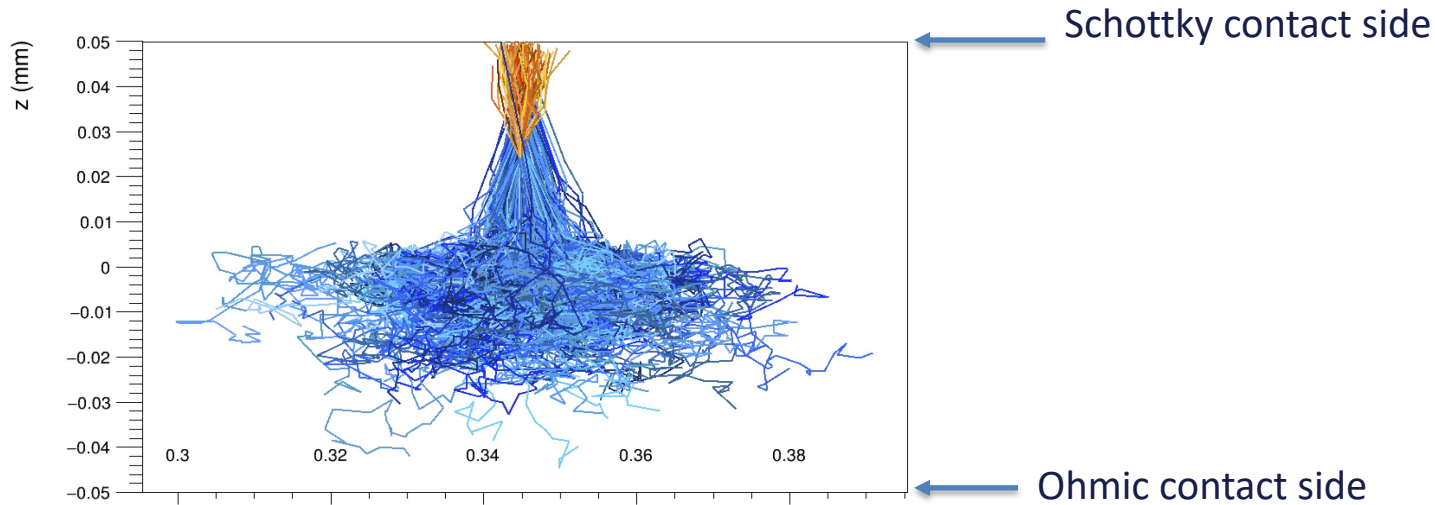
Charge (in 1,000s) created as a result of 5.486MeV alpha particles striking the top of a SiC detector ($z=185\mu\text{m}, x=0\mu\text{m}, y=0\mu\text{m}$) in a downward direction, 90 degrees to the surface of the detector



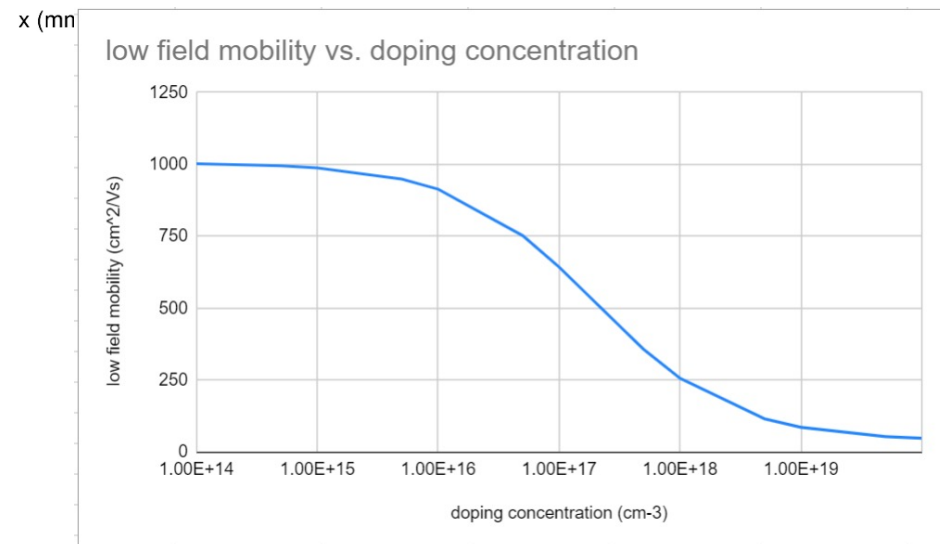
Charge (in 1,000s) created as a result of 5.486MeV alpha particles striking the top of a SiC detector ($z=185\mu\text{m}, x=0\mu\text{m}, y=0\mu\text{m}$) in a downward direction, 90 degrees to the surface of the detector.

Simulation results

✓ Charge propagation results



Charge propagation visual (holes in gold, electrons in blue), using Allpix² to graph the path taken by generated charge



Simulation results-illustration of electron/hole propagation

✓ Charge propagation visualization illustration

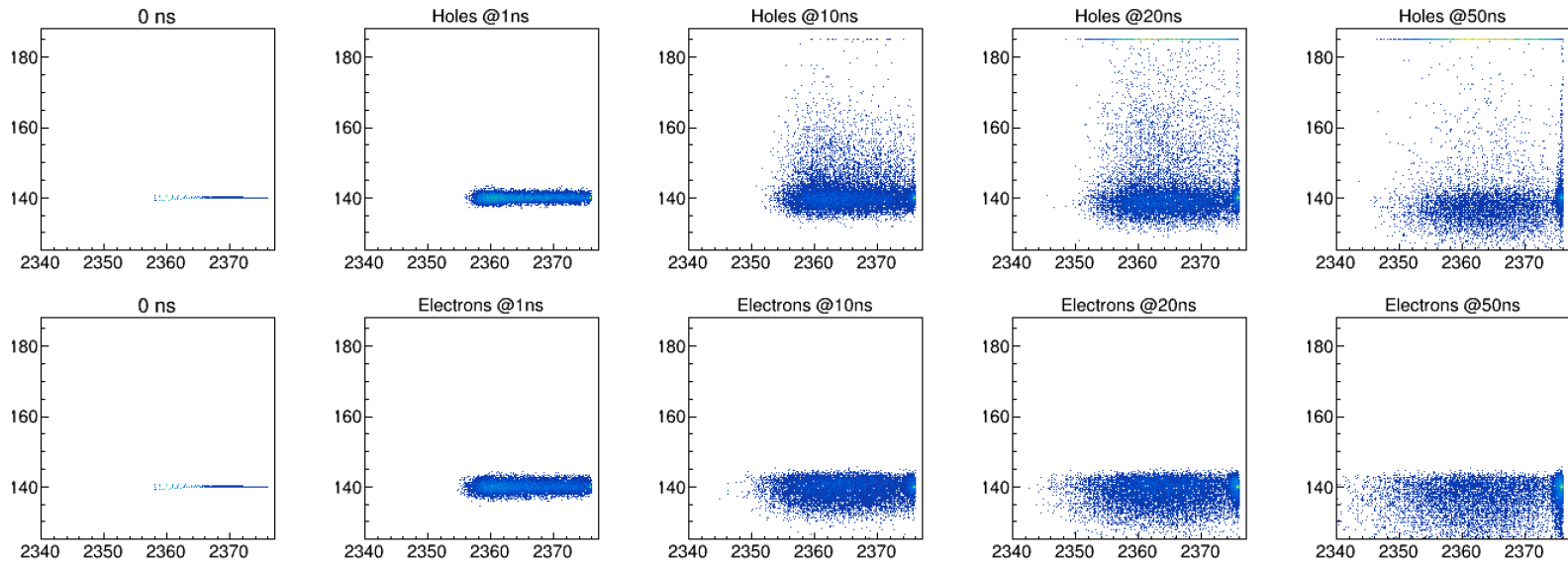
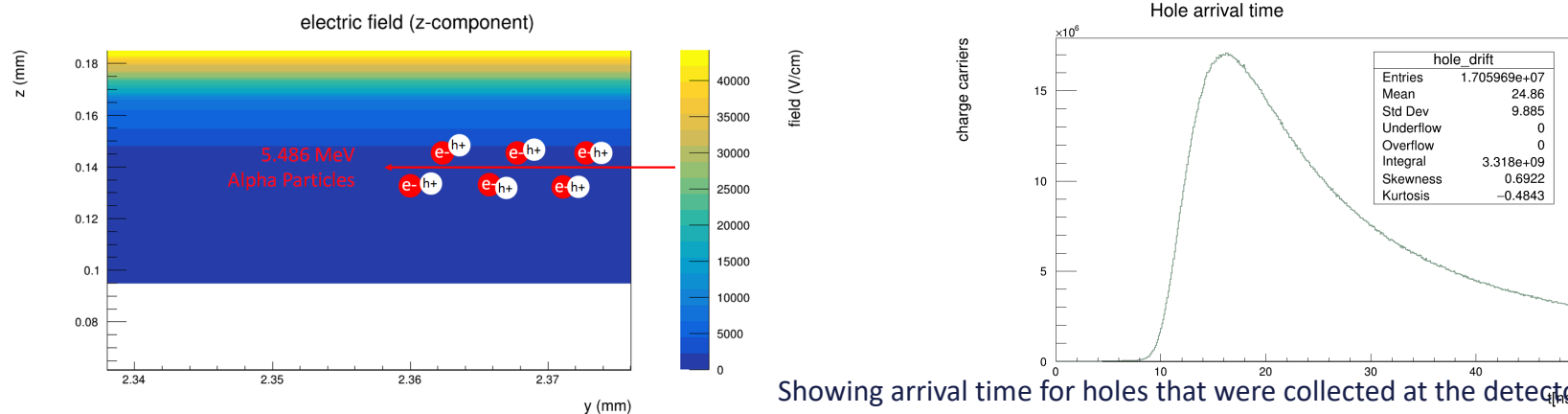


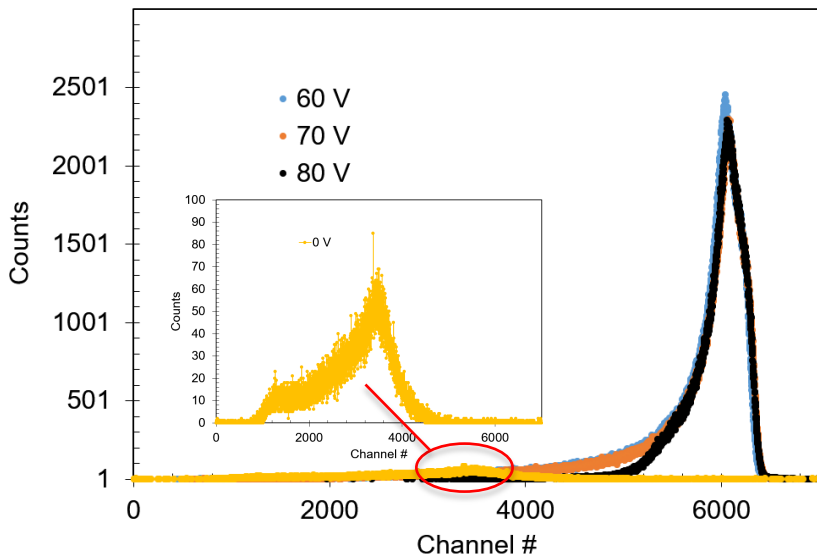
Figure 14 Charge propagation results, showing initial charge deposition location at 0 ns and various charge locations up to 50ns



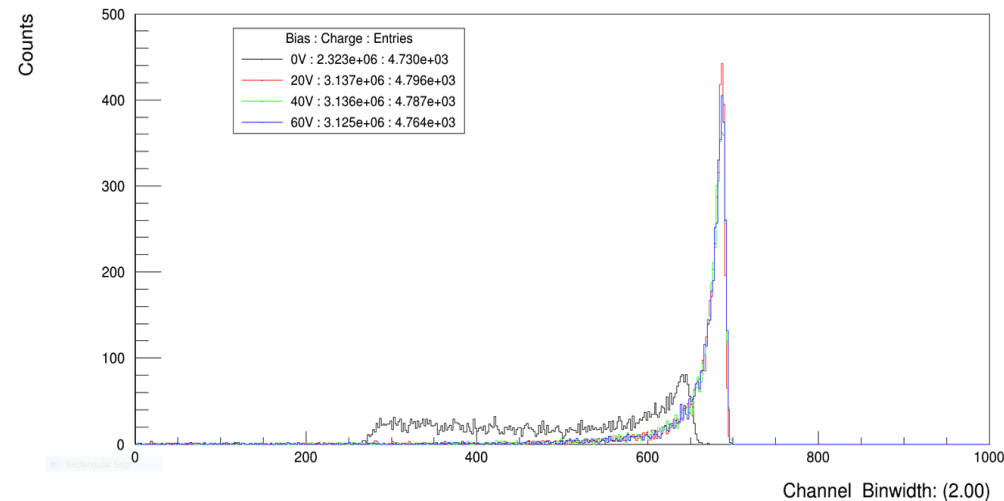
Showing arrival time for holes that were collected at the detector Schottky contact

Simulation-experimental results comparison

- ✓ The alpha spectra of the ^{241}Am plated SiC diode was acquired at different bias voltages and compared to the spectra simulated by Allpix² framework
- ✓ The default digitizer was used to generate the alpha spectrum of the device
 - Essentially, we need to compare the measured current generated by the ^{241}Am electrodeposited SiC device to the simulated results, however, due to the extremely low activity of the source (17 nCi), the measured current (pA level) from the device has large uncertainties as the device has a dark current of a few pA, therefore, the alpha spectra was simulated and compared to the acquired spectra instead



Experimentally acquired spectra of the ^{241}Am electrodeposited SiC device



Allpix² simulated alpha spectra of the device

Conclusion and outlook

- The alpha spectrum of an ^{241}Am electrodeposited SiC Schottky diode was simulated, and its charge carriers' propagation features were visualized by Allpix² simulation
- The experimentally acquired spectrum by the SiC diode shows good agreement with the simulated spectrum, indicating the effectiveness of using Allpix² framework for such simulations involving charge particles and the semiconductor devices
- This framework can be easily extended to a detailed nuclear-voltaic battery simulation, therefore, help to optimize the battery design

Thank you!



AwareAbility Technologies

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