Combining COMSOL and Monte Carlo Methods to Simulate SiC Sensors using the Allpix^2 Framework

Sha Xue[1], R. Gregory Downing[1], Vasil Hlinka[1], Daryl Giglio[2], Abigail Moore[1], Lei R. Cao[2]

1. AwareAbility Technologies, LLC, Columbus, Ohio

2. Nuclear Engineering Department, The Ohio State University, Columbus, Ohio

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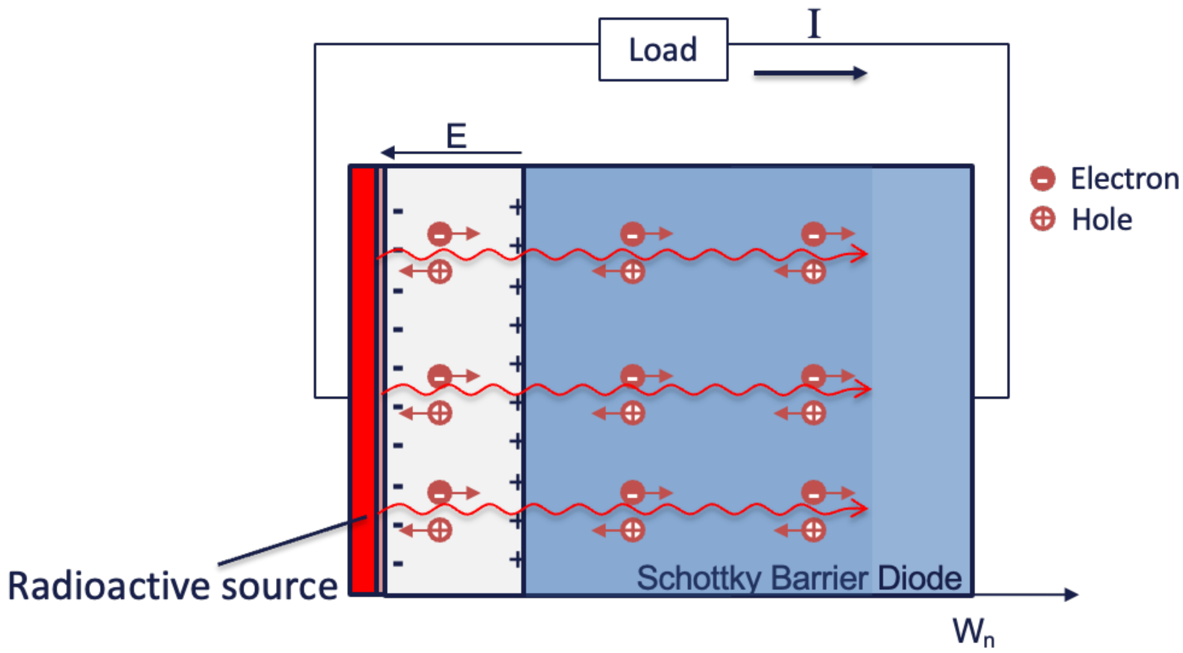
Introduction

- 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

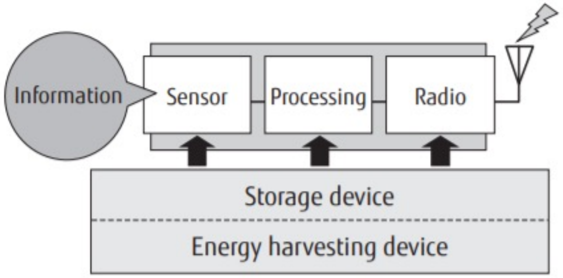
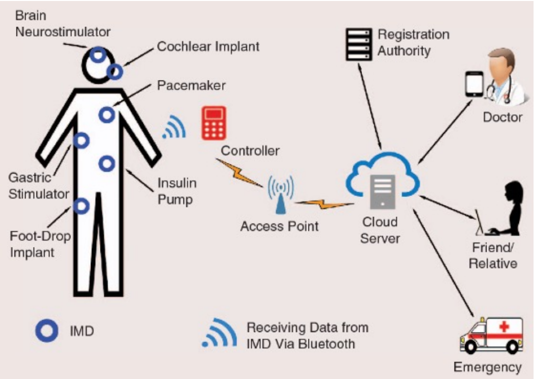


Figure 2
Self-powering wireless sensor module.
Tanaka, et al. Fujitsu Sci. Technol. J, 50, 93-100.

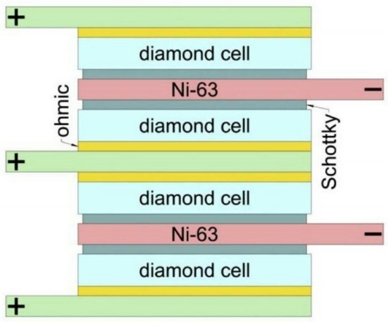
Maintenance free sensors

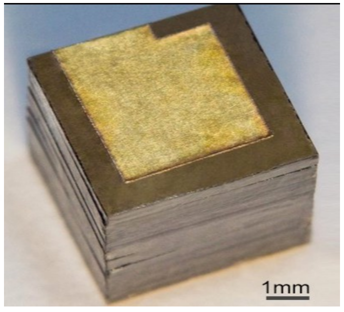


Implantable medical devices (IMD)

Introduction

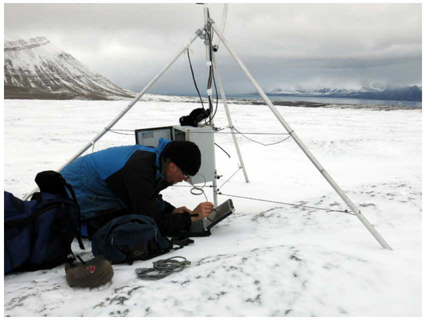
2) Flexible power output: (nW - μW)/single battery → meet different power demands by by stacking/scaling up

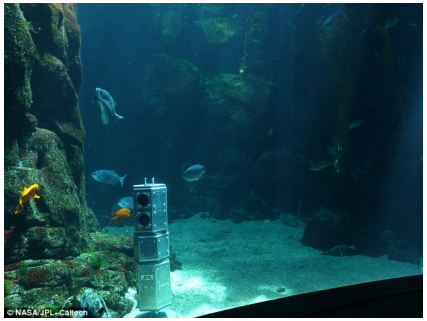




V. Bormashov et al./Diamond and Related Materials

3) Stable performance compared to chemical batteries





Extreme environment application

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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/cm^3) can be a disadvantage too

3) Radiation damage to the semiconductor material that could reduce the longevity of the battery

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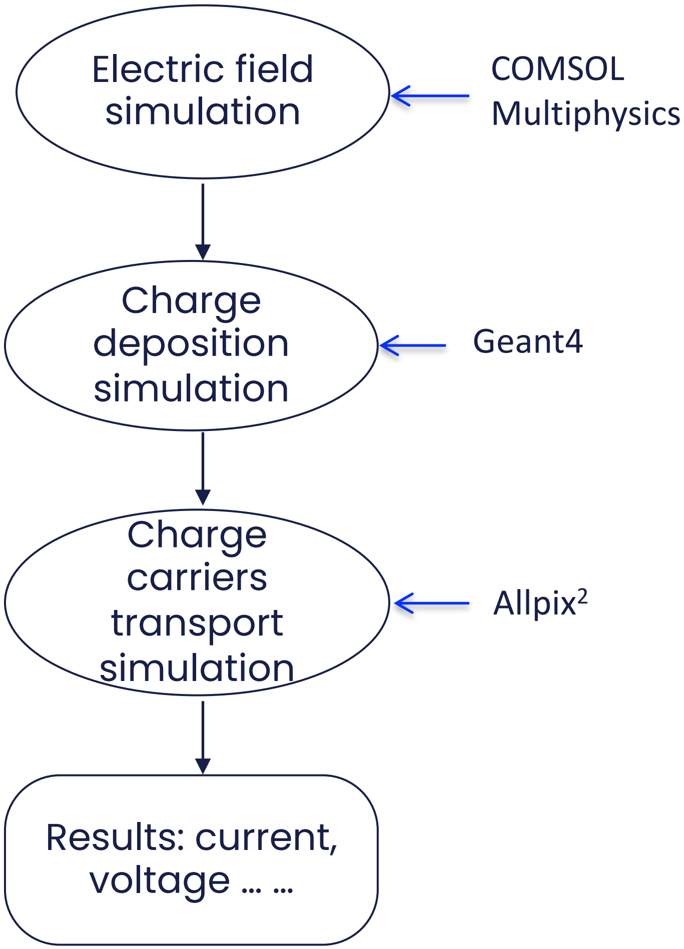
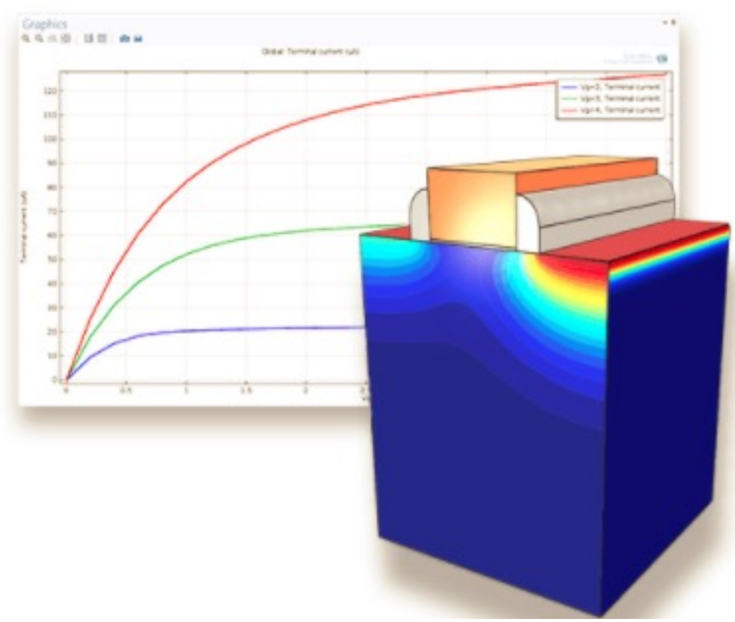
Motivation

- 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

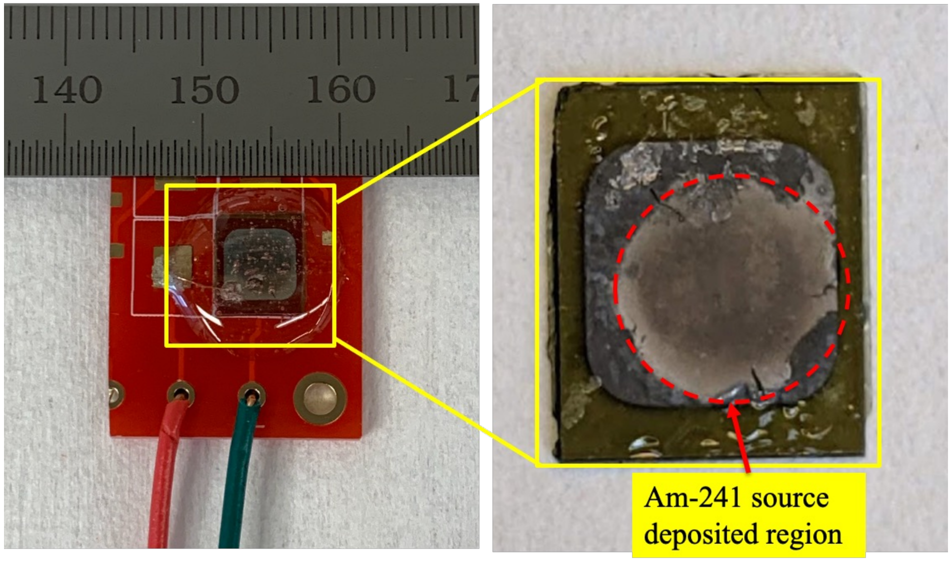


- Semiconductor modeling using the semiconductor module COMSOL Multiphysics:
  - Solves Poisson's equation in conjunction with the continuity equations for the charge carriers
  - Can simulate a wide range of semiconductor devices such as p-n junction, Schottky diodes, MOSFET, MESFET etc.



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)

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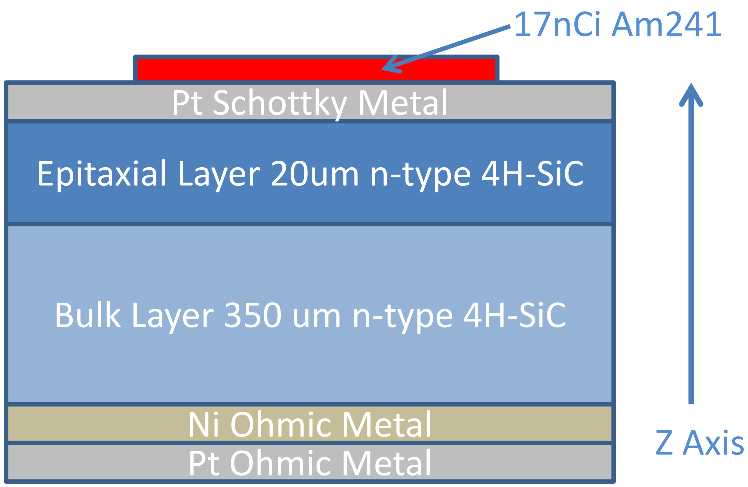
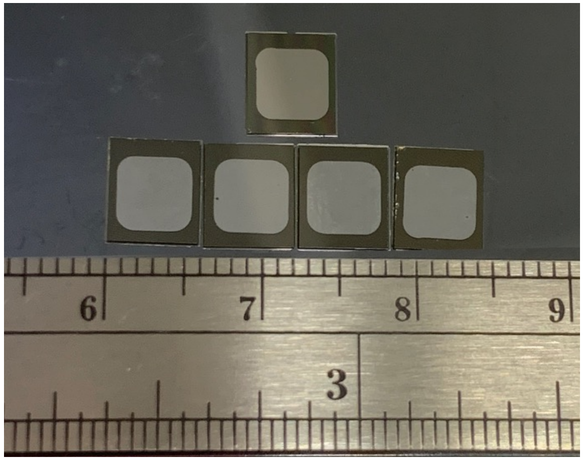
Device structure of the 4H-SiC Schottky diode

❖ 4H-SiC Schottky diode

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



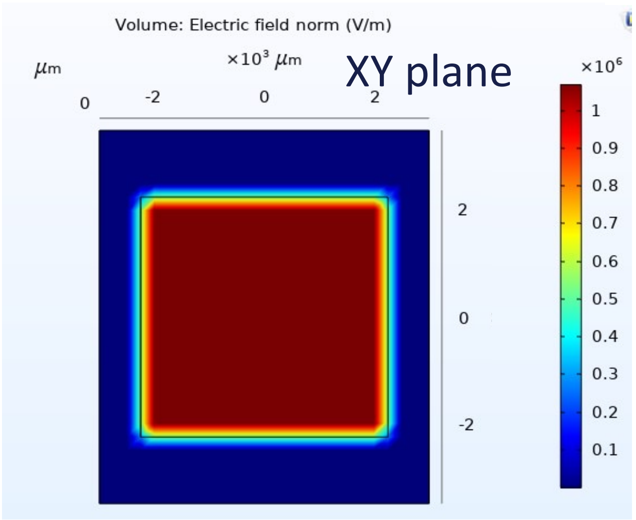
Schematic drawing of the Am-241 electrodeposited SiC Schottky diode

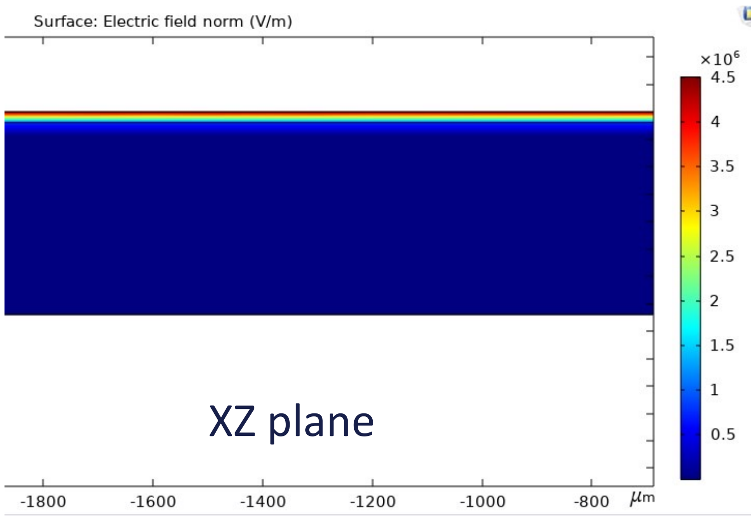


Custom fabricated Pt/SiC Shottky diodes prior to electrodeposition

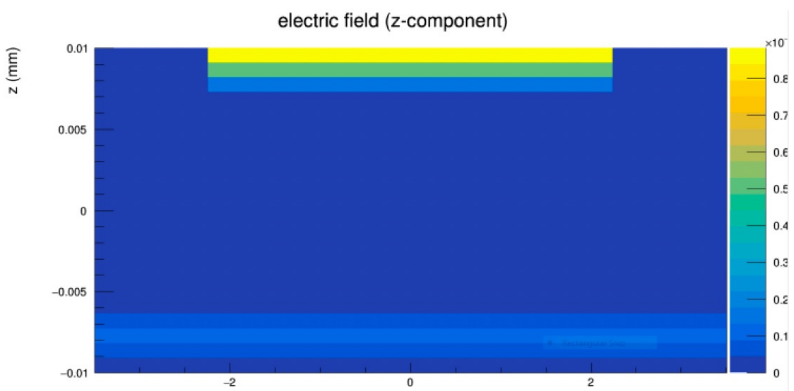
Electric field simulation of the 4H-SiC Schottky diode

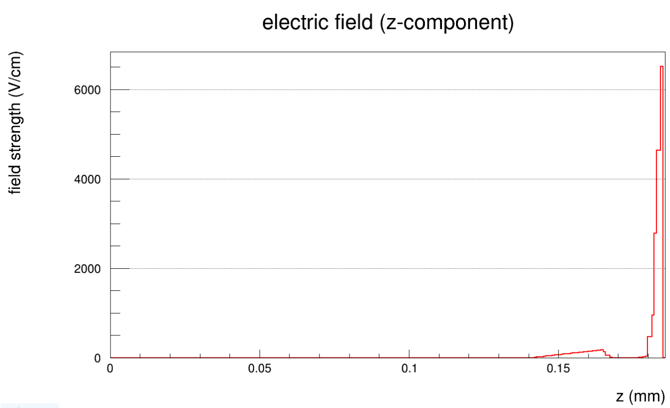
❖ Electrostatic simulation of the SiC Schottky diode





❖ Electric field results were imported to Allpix² using mesh converter





Electric field distribution in the z direction

Technologies

Charge carriers' mobility model

- ✓ The Caughey–Thomas approximation for the low-field carrier mobilities of 4H-SiC was implemented in the Allpix^2

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

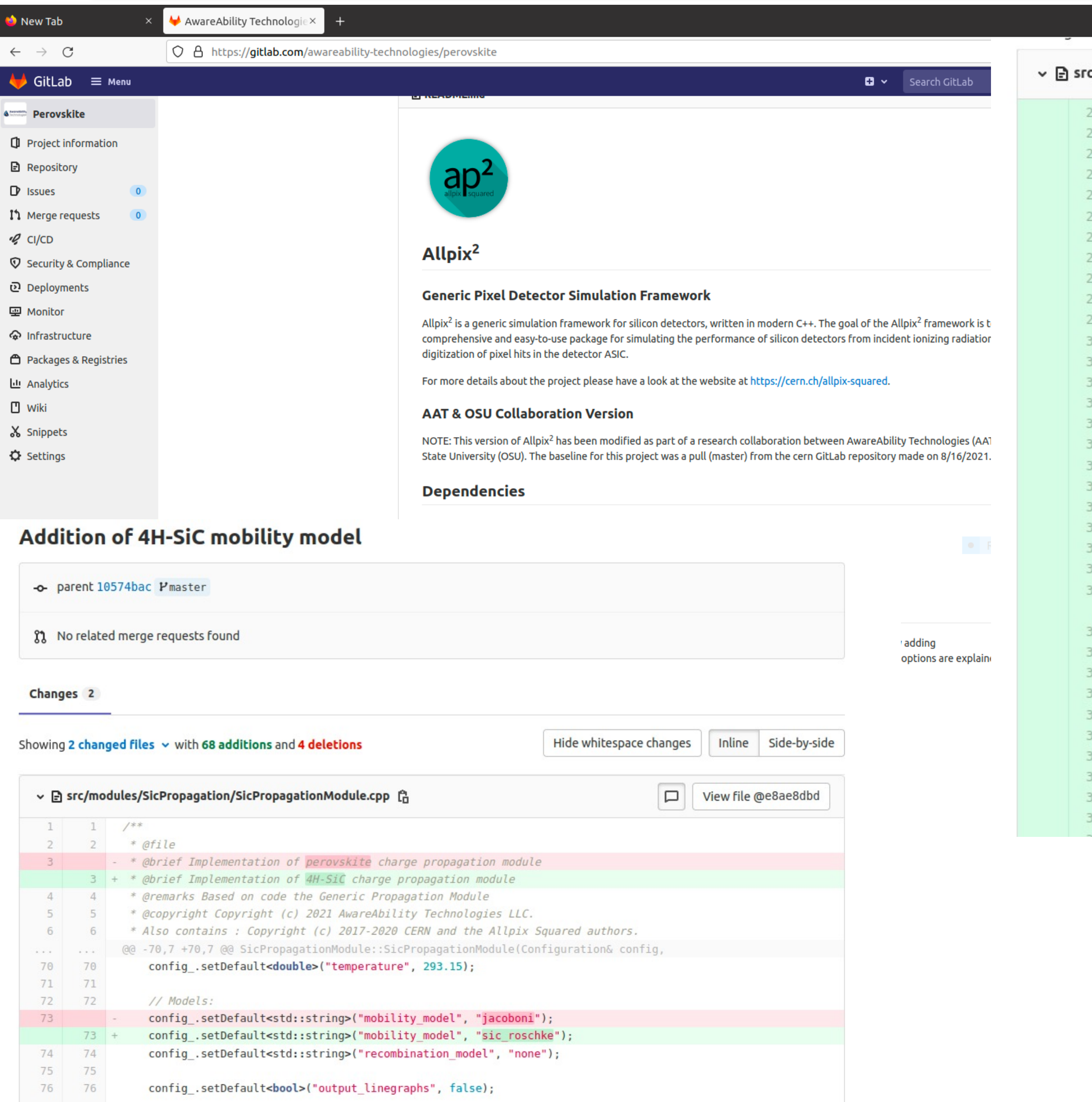
considering the temperature dependence of the parameters, the equation becomes

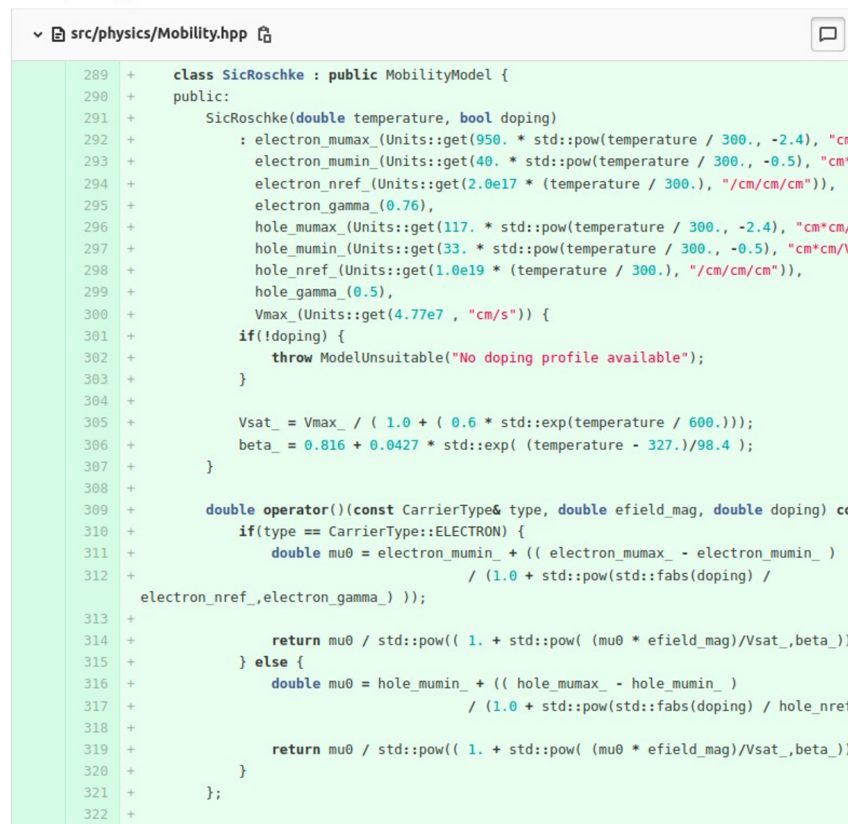
$$\mu_{n,p} = \mu_{n,p}^{min,0}\left(\frac{T}{300\mathrm{K}}\right)^{\alpha_{n,p}} + \frac{\mu_{n,p}^{max,0}\left(\frac{T}{300\mathrm{K}}\right)^{\alpha_{n,p}} - \mu_{n,p}^{min,0}\left(\frac{T}{300\mathrm{K}}\right)^{\beta_{n,p}}}{1 + \left(\frac{T}{300\mathrm{K}}\right)^{\gamma_{n,p}}\left(\frac{N_i}{N_{n,p}^{crit,0}}\right)^{\delta_{n,p}}}$$

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

Carrier type	$\mu^{min,0}$ $\mathrm{cm^2V^{-1}s^{-1}}$	$\mu^{max,0}$ $\mathrm{cm^2V^{-1}s^{-1}}$	$N^{crit,0}$ $\mathrm{cm^{-3}}$	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]

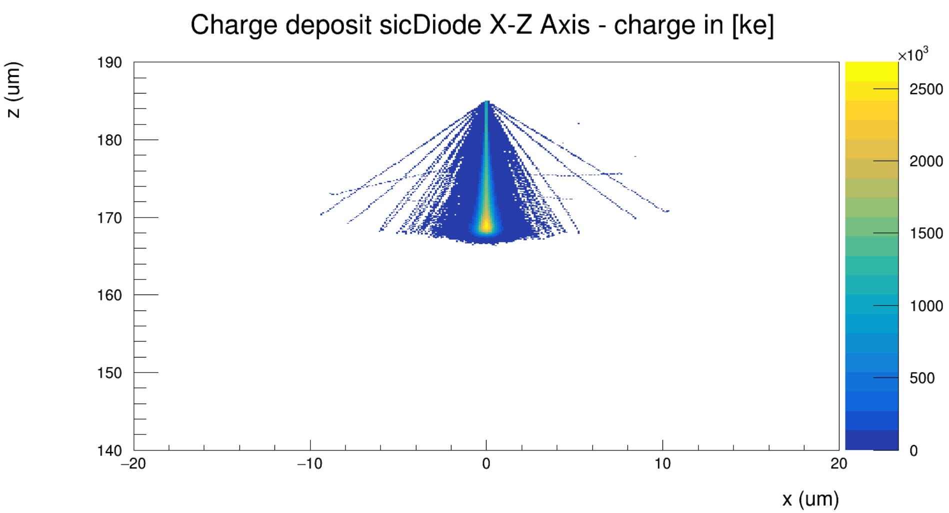
Charge carriers’ mobility model



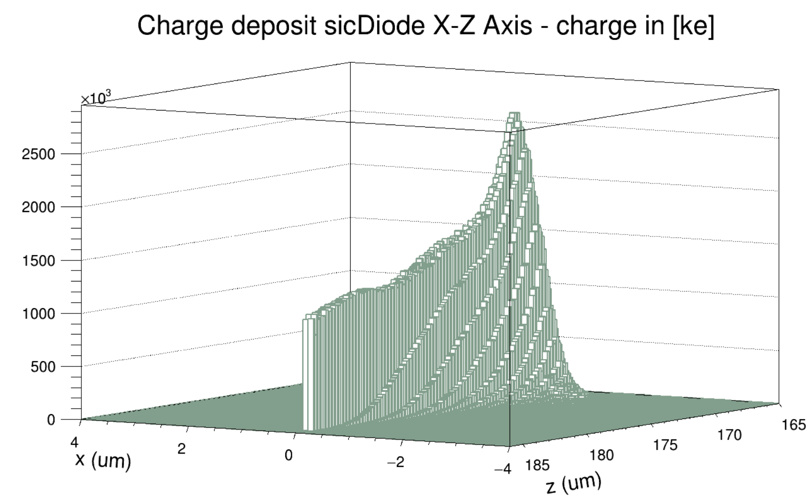


Simulation results-charge creation in the SiC sensor

✓ Charge deposition results



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

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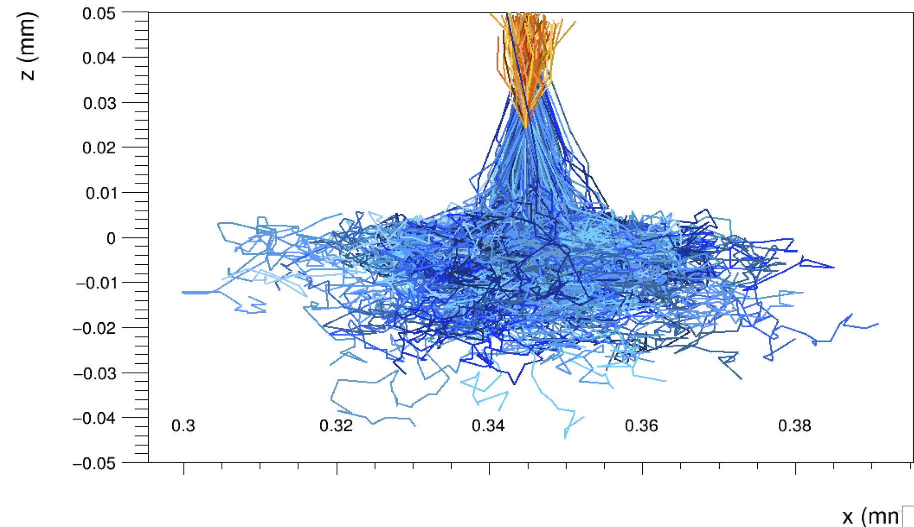
Simulation results

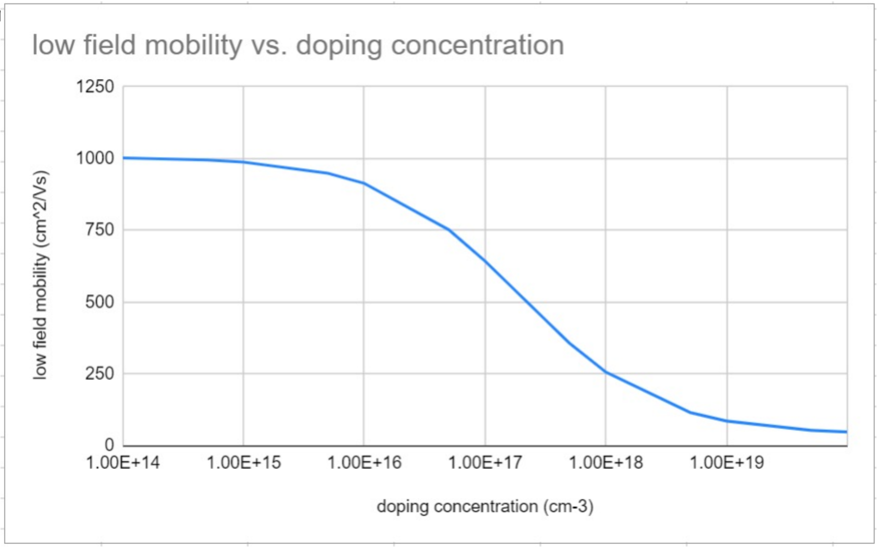
✓ Charge propagation results



Schottky contact side

Ohmic contact side

Charge propagation visual (holes in gold, electrons in blue), using Allpix^2 to graph the path taken by generated charge



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Simulation results-illustration of electron/hole propagation

✓ Charge propagation visualization illustration

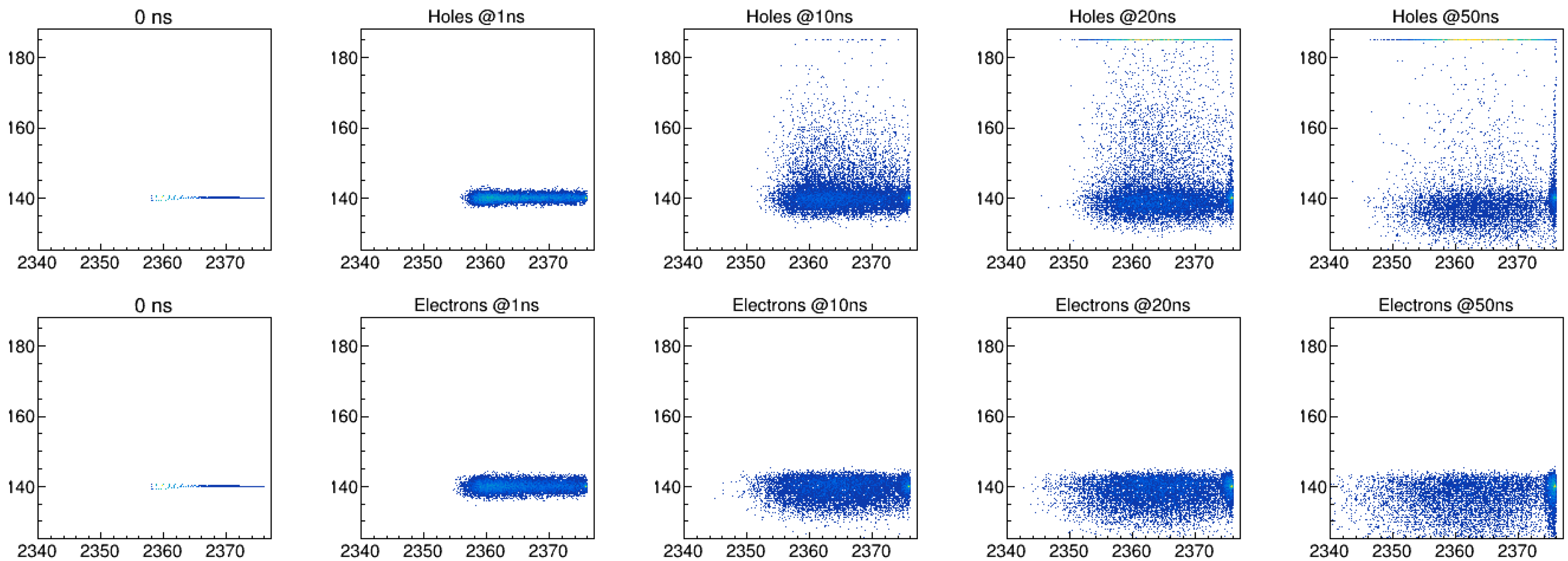
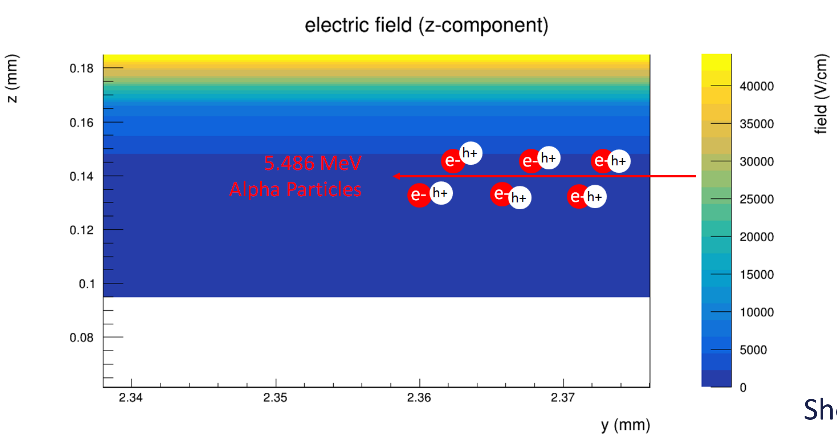
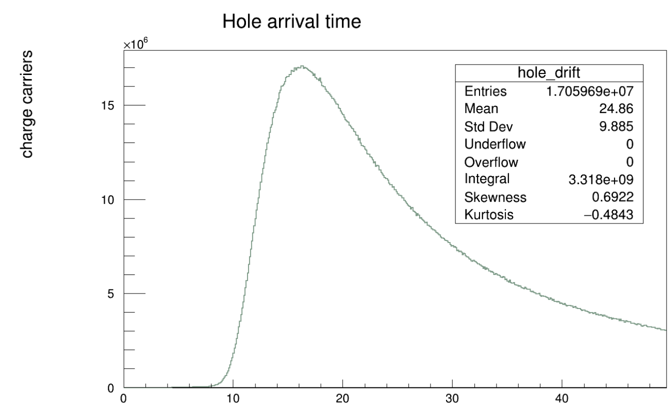


Figure 14 Charge propagation results, showing initial charge deposition location at 0 ns and various charge locations up to 50ns

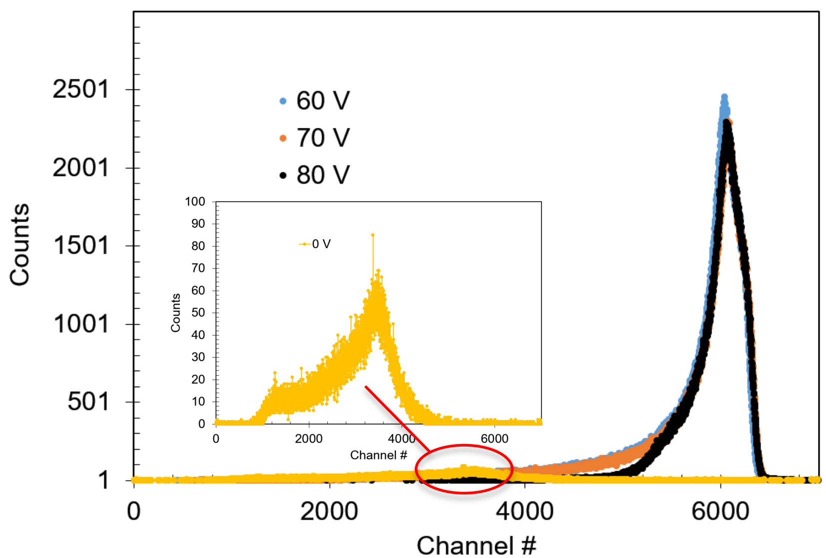




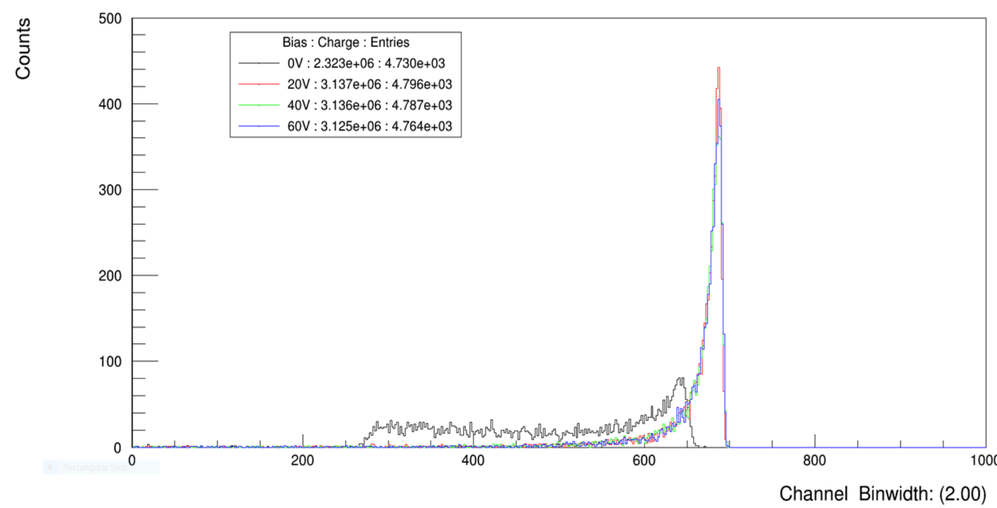
Showing arrival time for holes that were collected at the detector Schottky contact

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 Allpix^2 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



Allpix^2 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 Allpix^2 simulation
- The experimentally acquired spectrum by the SiC diode shows good agreement with the simulated spectrum, indicating the effectiveness of using Allpix^2 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

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Thank you!

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Name: Sha Xue
Email: sha.xue@Awaretk.com