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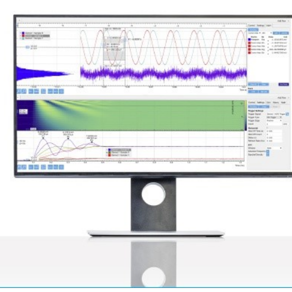

Simulation of Silicon Solar Cell Radiation Effects with GEANT4

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Abstract. In this paper we present the approach to numerical simulation of the radiation effects in Silicon solar cells with GEANT4 software. Improvements to solar cell radiation hardness are critical for power generation applications in long-term space missions. When solar cells are used in outer space or in Lunar environment, they are subject to bombardment by high-energy particles, which induce a degradation referred to as radiation damage. A family of predictive models for radiation effects induced by high energy protons in a silicon solar cell structure have been developed using a number of software tools [7]. Simulation of electron radiation effects in solar cells is equally required, but was still missing due the abbsence of the software. GEANT4 is a software toolkit for the simulation of the passage of particles through matter. GEANT4 has both electron and proton radiation simulation capability, that makes it attractive to apply to solar cells simulation. Performed and presented in this paper numerical experiments demonstrate that GEANT4 can be used for simulation of silicon solar cell radiation effects, that was not possible before with other software.

INTRODUCTION

Improvements to solar cell efficiency and radiation hardness that are compatible with low cost, high volume manufacturing processes are critical for power generation applications in future long-term NASA and DOD space missions. When solar cells are used in outer space or in Lunar or Marsian environments, they are subject to bombardment by high-energy particles, which induce a degradation referred to as radiation damage. Radiation tolerance (or hardness) of this ultra-thin (UT) Si photovoltaic technology (PV) is not well understood. Experimental investigation of the radiation effects in solar cells are very expensive and time consuming. Therefore, we will use the physics-based simulation approaches to investigate the radiation effects in ultrathin Si solar cell technology, to improve the radiation hardening of those before starting the costly experiments. The simulation tools for UT Si PV cell technologies, will help to: (a) assess technologies, devices, and materials for more efficient Si photovoltaic solar cells; (b) better evaluate the performance and radiation response at early design stage; (c) set requirements for hardening and testing; reduce the amount of testing cost and time. Our past approach to numerical simulation of the radiation effects in Si PV cells subject to proton irradiation, resulted in developed of a family of predictive model for radiation induced effects by high energy protons in a silicon solar cell structure [6] , [16], [7] , [8], [12], [13], [22], [23]. A number of different software tools have been used, including the SRIM software [21], ITS software [14], CASINO [5], and different TCADs [8]. None of these codes do the necessary electron irradiation simulations. Some limited capabilities are available in the CASINO [5] software, still that has very limited capabilities for our purpose, as it is mainly designed for the Scanning Electrone Microscope (SEM). The following sections will overview the electron irradiation simulation approaches for solar cells and simulation results.

SIMULATION OF SILICON SOLAR CELLS SUBJECT TO ELECTRON RADIATION

CASINO Code

CASINO as a well known electron irradiation simulation code, this is a Monte Carlo based simulation of electron trajectory in solids. This complex single scattering Monte Carlo program is specifically designed for low energy beam interaction in a bulk and thin foil, and can be used to generate many of the recorded signals (X-rays and backscattered

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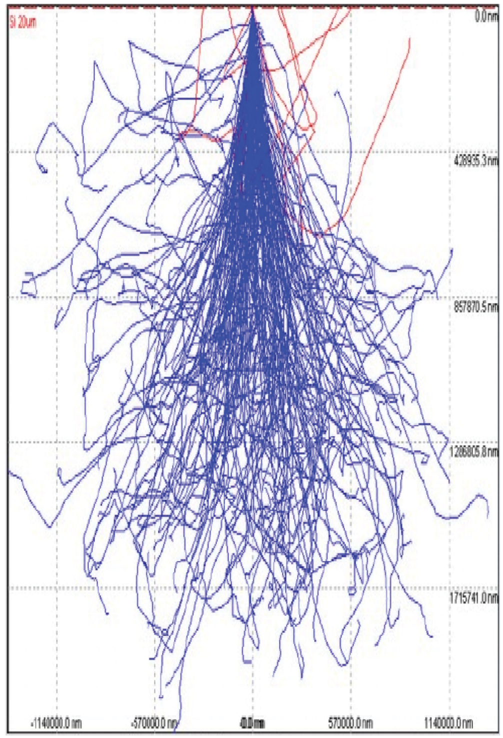


FIGURE 1. CASINO simulations of 1MeV electron irradiation of Si block: electron tracks, original beam electrons are shown by blue color, backscattered are shown by red color

electrons) [5]. The simulation results of 1MeV electron irradiation of large size Si block, that we have performed, are shown in Figure 1. One can see that 1MeV electrons are fully absorbed in Si within 2E6 nm range (2 mm).

The simulation results of 1MeV electron catholuminescence in large Si block are shown in Figure 2. We can see that it starts at about 200um and drops completely beyond 2mm depth. This gives us an estimate for the location of the Bragg peak at 200um of further (compare to 240um for 5MeV protons [8]).

PHYSICS BASED RADIATION EFFECT MODELS

Figure 3 presents the experimental stopping power (dE/dX) of electrons in Si [NIST]. It has minimum at the energy of interest, 1MeV, $dE/dx \sim 0.5\mathrm{keV/um}$. This gives us an estimate for the stopping range of 1MeV electrons in Si at 2000μm=2mm), and compares well with our CASINO simulations result of 2mm.

The drawbacks of CASINO code are the following:

- No source code available, therefore neither development nor extension of the software are possible.
- Post-processing of results is very limited, no material defect data are available/possible.
- This code is for electron trajectories visualization only, mainly for SEM device applications purpose.

A subsequent model development involves the GEANT4 radiation simulation tool, developed at Stanford University, which look as the most appropriate for accurate physics of defect creation and identification in the Si material [Geant4].

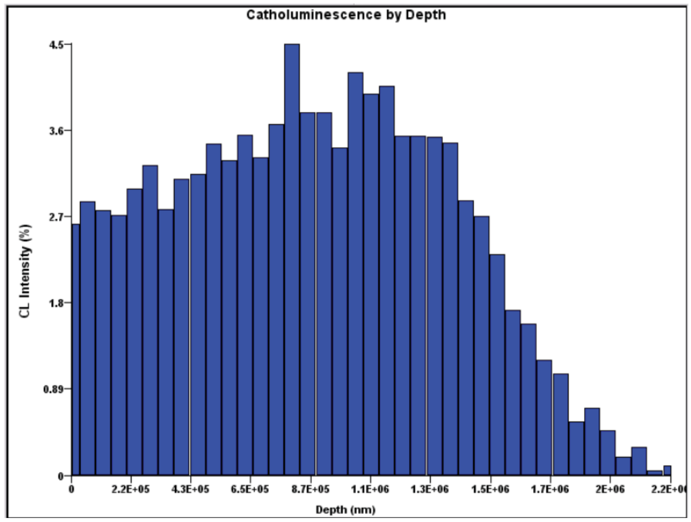


FIGURE 2. CASINO simulations of 1MeV electron irradiation of Si block: catholuminiscence starts at about 200um and drops completely beyond 2mm depth. This gives us an estimate for the location of the Bragg peak beyond 200um (compare to 240um for 5MeV protons [8])

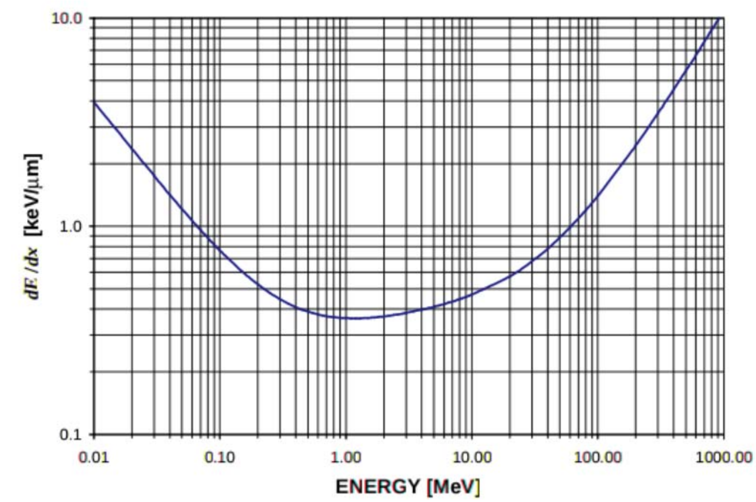


FIGURE 3. The stopping power (dE/dX) of electrons in Si: it is minimal at 1MeV, dE/dx 0.5keV/um [20]. This gives us an estimate for the stopping range of 1MeV electrons in Si at 2000um=2mm). This compares very well with our simulations result of 2mm.)

GEANT4 Software Toolkit

GEANT4 is a software toolkit for the simulation of the passage of particles through matter. It is used in large number of experiments and projects, in a variety of application domains, including high energy physics, astrophysics and space science, medical physics and radiation protection [4], [3], [2], [1], [17]. Over the past several years, major changes have been made to the toolkit in order to accommodate the needs of these user communities, and to efficiently exploit the growth of computing power made available by advances in technology [18], [19]. The adaptation of GEANT4 to multithreading, advances in physics, detector modeling and visualization, extensions to the toolkit, including biasing and reverse Monte Carlo, and tools for physics and release validation are discussed in [4]. Indeed, GEANT4 simulation has become mission-critical in fields such as high energy physics and space science. It has been created exploiting software engineering and object-oriented technology and implemented in the C++ programming language.

The key domains of the simulation of the passage of particles through matter implemented in Geant4 are:

- geometry and materials;
- particle interaction in matter;
- tracking management;
- digitization and hit management;
- event and track management;
- visualization and visualization framework;
- user interface.

Geant4 gives to the user full freedom and a full control of the code design and execution for a particular problem (C++ programming is a must). A wide range of particles is available, including the key particles of interest for solar cells irradiation: electron and proton. Available physics models can be used, and new physics models can be designed and incorporated in the Geant4 for a particular application (in C++ language).

GEANT4 Based Simulations

The overall goal of the work was to enable Geant4 simulation capabilities for accurate solar cell electron radiation effects to improve the solar cell efficiency and radiation hardness, by the proper choice of the solar cell material composition, and design to mitigate radiation effects and solar cell degradation.

The long reaching goals include the following:

- Reproduce the key relevant simulations for semiconductor material radiation effects available in GEANT4 library, to ensure the correctness and accuracy of simulations.
- Enable GEANT4 low energy "semiconductors" component for accurate simulation in the energy range from 0.1eV to 10MeV, as typical applications of GEANT4 in HEP have the energy range from 10MeV to 200TeV [18].
- Set up typical geometry and material composition for Si solar cell in Geant4, and radiation sources, and conduct electron irradiation experiments simulations with Geant4 (that were not possible to complete with IAS Tiger series; SRIM; and CASINO software).
- Evaluate the results and graphical representation of solar cell radiation effects: displacement damage, composition of material post radiation and distribution of the defects (vacancies, ionization, interstitial, and phonon production in the target material).
- Predict of the formation of particular defects (like BiOi) in the target material depending on the composition (doping, oxygen) and temperature.
- Calculate radiation induced defects (traps) energy levels and cross-sections, depending on the solar cell material/composition.
- Evaluate the capability of predicting the solar cell annealing process, based on simulations.

GEANT4 Software Architecture Selected

The Geant4 virtual machine

To minimize the installation efforts, we have chosen the Geant4 Virtual Machine (VirtualBox VM), that provides a compiler, the extra software which Geant4 requires including a large set of visualization libraries, and a fully working Geant4 system. It avoids the effort to find and install the key pieces needed to create an installation on your own system, which varies depending on the OS, its version and many other factors. Further details can be found at the

CENBG home of the Geant4 Virtual Machine. The VirtualBox version was downloaded with GEANT4.10.05 at `ftp://ftp.cenbg.in2p3.fr/info/Vmware/geant4.10.05/VirtualBox/`.

Electron irradiation simulation with Geant4

Basic examples have been provided to start test cases and to develop the user application, in form of C++ codes, GUI scripts, *etc.* Example B1 described in [Allison 2016], has been compiled and ran successfully, see Figure 4.

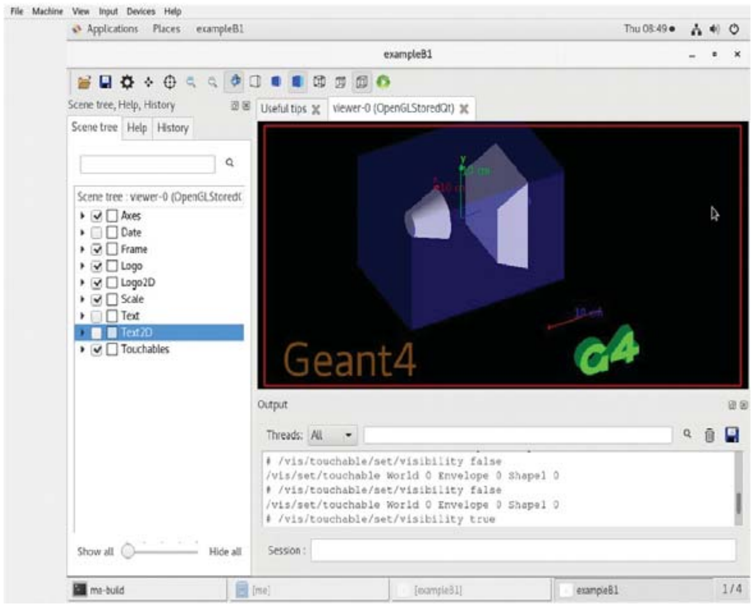


FIGURE 4. The GEANT4 demonstration of the capability of 3D radiation energy deposit in different volumes. GUI and graphics are shown running in VirtualBox Centos7 in Linux OS desktop.)

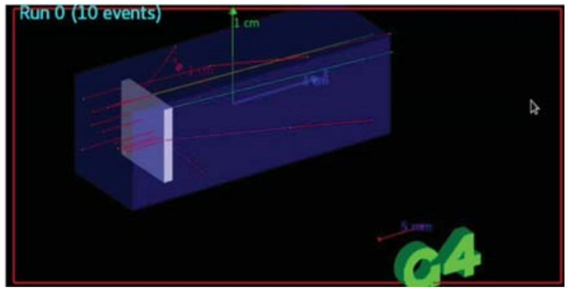
Simulation of Electron Irradiation in Si

This case followed by Si wafer electron irradiation experiment, developed from B1, and presented in Figure 5: 1mm thick Si wafer electron irradiation experiment, (a) and (b), and (c) for 100 micrometer thick Si wafer and 100 electron events.

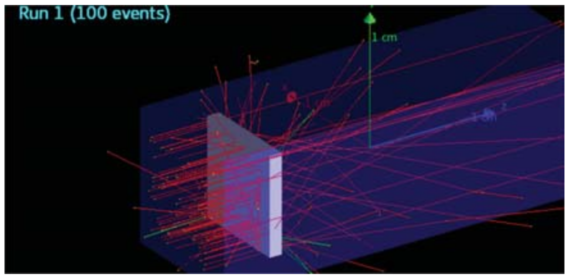
Analysis of Electron Irradiation with Geant4

The microelectronics example illustrates the possibility to combine discrete and condensed history processes in Geant4 at different geometrical scales and in selected regions in a unique Geant4 application, thanks to the common software design adopted by the electromagnetic physics working group of the Geant4 collaboration. It utilizes the physics models that are accurate at low energies (below 10MeV). It simulates the track of a 5MeV proton in silicon. Geant4 standard EM models are used in the World volume while Geant4-MicroElec models are used in a Target volume, declared as a Region. Instead we set the electron gun for 1MeV and changed the target – Si wafer – to the UT Si PV dimensions: 20um $\times$ 20um $\times$ 10um thick, see Figure 7 for geometry. The simulation ran for 100,000 electrons and the hystogramm of the physical processes involved is shown in Figure 7. The only particle is e- , and processes occurred are marked by flags:

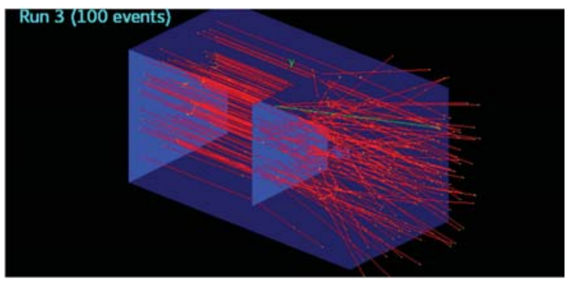
```
Processes name  Flag:
e-_G4MicroElecElastic 11
e-_G4MicroElecInelastic 12
eCapture 13
p_G4MicroElecInelastic 14
```



(a)



(b)



(c)

FIGURE 5. The GEANT4 simulation of 1mm thick Si wafer electron irradiation experiment, (a) ten electron generated by the electron gun (on a left), and (b) 100 electrons,(c) 100 micrometer thick Si wafer and 100 electron events

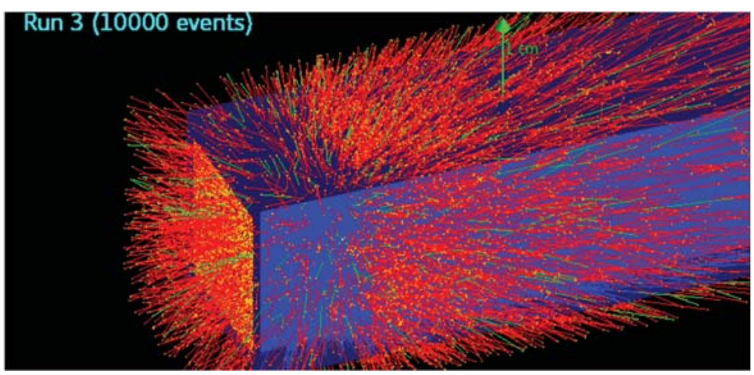


FIGURE 6. The GEANT4 simulation of 1mm thick Si wafer electron irradiation experiment, 10,000 electron events

```
ion_G4MicroElecInelastic 15
Processes name  Flag:
hIoni 16
eIoni 17
```

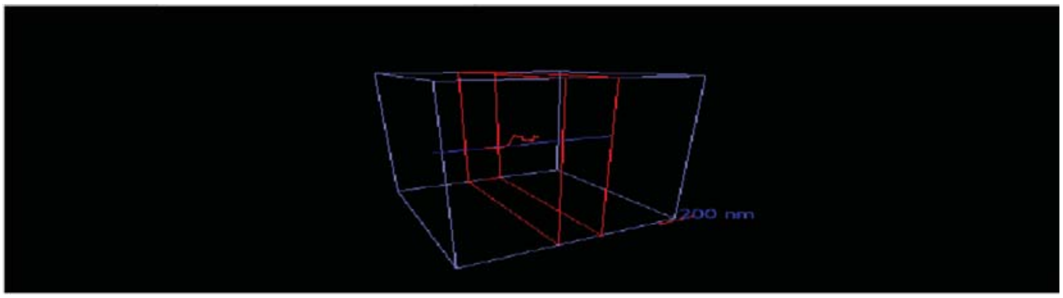


FIGURE 7. The GEANT4 simulation of 10um thick Si wafer electron irradiation experiment, using the accurate low energy physics models from "microelectronics" library: geometry setup is shown

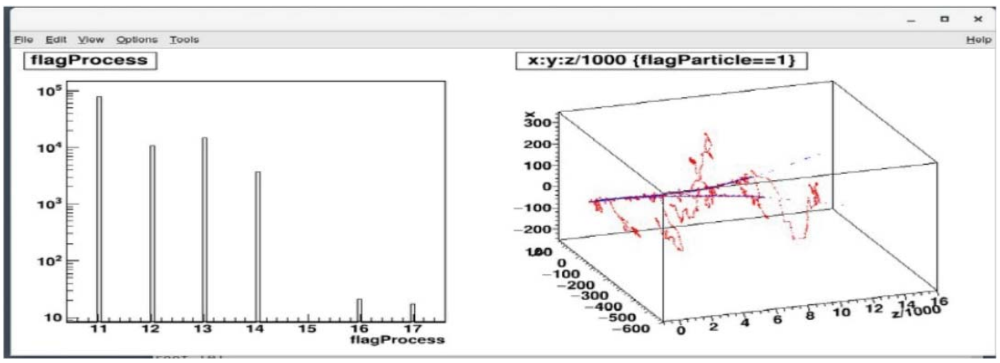


FIGURE 8. The GEANT4 simulation of 10um thick Si wafer electron irradiation experiment, and processing the statistics with ROOT graphics software: processes involved by flag number, and geometry setup

CONCLUSION

Summary on GEANT4 simulation of electron radiation effects is the following:

- Installation and testing of the the GEANT4 virtual machine and software have been successfully completed.
- GEANT4 low energy "semiconductors" component have been tested for more accurate simulation of radiation effects in the low energy range from 0.1eV to 10MeV, compared to the standard GEANT4 distribution.
- The procedure of Seting up typical geometry and material composition for Si solar cell in Geant4, and radiation sources has been successfully accomplished.
- Successfully conducted electron irradiation experiments simulations with Geant4 (that were not possible in a past with other software).
- The results are quite encouraging, and will be advanced in future work.

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