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Beta particle transport and its impact on betavoltaic battery modeling

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HIGHLIGHTS

- The impact on beta particle penetration depth and energy deposition for betavoltaic battery design are studied using MCNP.
- Different beta particle transport approaches are examined for betavoltaic battery by junction depth analysis.
- An isotropic source needs to be considered in the beta particle transport model.
- The inclusion of the self-absorption effect improves the betavoltaic battery model significantly.

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ABSTRACT

Simulation of beta particle transport from a Ni-63 radioisotope in silicon using the Monte Carlo N-Particle (MCNP) transport code for monoenergetic beta particle average energy, monoenergetic beta particle maximum energy, and the more precise full beta energy spectrum of Ni-63 were demonstrated. The beta particle penetration depth and the shape of the energy deposition varied significantly for different transport approaches. A penetration depth of 2.25 ± 0.25 μm with a peak in energy deposition was found when using a monoenergetic beta particle average energy and a depth of 14.25 ± 0.25 μm with an exponential decrease in energy deposition was found when using a full beta energy spectrum and a 0° angular variation. For a 90° angular variation, i.e. an isotropic source, the penetration depth was decreased to 12.75 ± 0.25 μm and the backscattering coefficient increased to 0.46 with 30.55% of the beta energy escaping when using a full beta energy spectrum. Similarly, for a 0° angular variation and an isotropic source, an overprediction in the short circuit current and open circuit voltage solved by a simplified drift-diffusion model was observed when compared to experimental results from the literature. A good agreement in the results was found when self-absorption and isotope dilution in the source was considered. The self-absorption effect was 15% for a Ni-63 source with an activity of 0.25 mCi. This effect increased to about 28.5% for a higher source activity of 1 mCi due to an increase in thickness of the Ni-63 source. Source thicknesses of approximately 0.1 μm and 0.4 μm for these Ni-63 activities predicted about 15% and 28.5% self-absorption in the source, respectively, using MCNP simulations with an isotropic source. The modeling assumptions with different beta particle energy inputs, junction depth of the semiconductor, backscattering of beta particles, an isotropic beta source, and self-absorption of the radioisotope have significant impacts in betavoltaic battery design.

1. Introduction

Betavoltaic batteries harvest energy from beta emitting radioisotope sources using semiconductors. The kinetic energy of the beta particles from the radioisotope is converted into electrical energy in the semiconductor. Betavoltaic batteries have some unique features such as a long service life (several years to several decades) and small size (Kwon and Robertson, 2009; Lal and Blanchard, 2004). They can be miniaturized to micron sizes due to their high energy density. These advantages of betavoltaic batteries over other types of batteries make them an attractive power source for fulfilling the requirements of future generation electronic devices (Wu et al., 2011; Prelas et al., 2014).

This work examines and contrasts the strengths and weaknesses of the main modeling philosophies applied to betavoltaic batteries. The analysis of the energy deposition of beta particles in semiconductors, the estimation of their penetration depth, and the profile of electron-hole pair (EHP) generation in semiconductors are of utmost importance in betavoltaic battery design. These analyses are important in order to get a better estimate of EHP production, which determines the semiconductor design parameters such as top layer thickness or junction

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depth, doping concentrations, and thickness. The design of the battery varies depending on how the beta particle energy is chosen such as average beta particle energy or the full beta energy spectrum, beta particles angular emission such as isotropic or non-isotropic emission, and the consideration of self-absorption effects (Prelas et al., 2016). Many researchers have used different methods such as the Katz-Penfold range equation, the Everhart and Hoff range equation, the Kanaya-Okayama model, and Monte Carlo methods such as Monte Carlo N-Particle (MCNP) transport code for determining energy deposition and penetration depth (Alam and Pierson, 2016; Ulmen et al., 2009; Thomas et al., 2016; Alam et al., 2015). Most of the available betavoltaic designs have only considered the average beta particle energy. The Monte Carlo method using MCNP software (Goorley, 2012) was used in this work because of its comprehensive atomic physics model which obtains better estimates of energy deposition and penetration depth. Monoenergetic beta particle average energy, monoenergetic beta particle maximum energy, and a full beta energy spectrum of Ni-63 were considered as different types of source inputs in the MCNP model to analyze the energy deposition and penetration depth in silicon (Si). Some recent works showed the qualitative difference in energy deposition for different beta input energies and discussed the importance of modeling full beta energy spectrum (Zuo et al., 2013; Zaitsev et al., 2014; Gui et al., 2016; Polikarpov and Yakimov, 2015; Yakimov, 2016). In this work, it will be shown that different input energy profiles could have a significant impact on betavoltaic battery design based on the junction depth analysis. The penetration depths obtained from the MCNP model and the Katz-Penfold range equation for monoenergetic beta particle average energy and monoenergetic beta particle maximum energy of Ni-63 in Si were compared. The MCNP model was further analyzed for different angular distributions of the beta particle's initial direction for a full beta energy spectrum. In reality, beta particles are emitted isotropically from a radioisotope source. It will be shown that the variation in angular distribution of the beta particles is an important factor for betavoltaic battery design. The analysis of a backscattering effect due to various angular emissions of beta particles has significant impact in the design. A simplified drift-diffusion semiconductor model was then used to calculate the short circuit current, the open circuit voltage, and the leakage current for the betavoltaic batteries. It was shown that the junction depth is a very important design parameter in determining the short circuit current, open circuit voltage, and leakage current. However, the optimum junction depth depends on the beta particle energy input and its angular distribution. The simulated betavoltaic battery results were then compared to some results from the literature for actual betavoltaic batteries. The results were explained by the self-absorption effect of the beta particles in the radioisotope source. The self-absorption has normally been overlooked in the theoretical modeling of betavoltaic battery design. In reality, the efficiency of a betavoltaic battery is limited by the self-absorption effect of the radioactive source. Therefore, consideration of the self-absorption effect will provide a better estimate of betavoltaic battery outputs such as the short circuit current, open circuit voltage, and leakage current. It was noted that Zuo et al. also modeled Ni-63 with silicon and validated their results. However, the detailed studies and analyses of beta particles angular emission, backscattering effect, penetration depths, self-absorption effect, and the importance of optimum junction depth are presented in this work. Furthermore, the self-absorption effect of the source was analyzed using MCNP and compared with the results obtained by the chord method (Gui et al., 2016).

The organization of the paper includes a brief summary of the MCNP method and a brief discussion of the beta particle energy spectrum used in this work. It also includes the statistical reliability analysis of the MCNP outputs for convergence. Finally, the important effects of the penetration depth, EHP estimates, angular variation, junction depth, and self-absorption on the short circuit current, open circuit voltage, and leakage current are presented and discussed and then conclusions are drawn.

2. Method

The electron-photon-positron transport feature of MCNP6 (version Beta 3) was used in this work. MCNP uses a detailed physics model of electron-photon-positron transport. The physical events for electron transport are elastic and inelastic collisions of the incoming electrons (beta particles) emitted from a radioisotope source with the atomic electrons and nuclei in the material. An electron mainly loses its energy by inelastic collisions with the atomic electrons and changes direction by elastic collisions with the electrostatic field of the atomic nuclei (Evans, 1955; Zerby and Keller, 1967). The inelastic collisions with orbital electrons dominate at lower kinetic energies such as less than 10 MeV. In this case, the energy is lost due to atomic excitation and ionization, which in turn creates soft x-rays and knock-on electrons. When the electron energy is higher than a few MeV, the inelastic collisions with both atomic nuclei and electrons become dominant, which causes sudden speed changes in the incoming electrons. In this case, the energy is lost due to the bremsstrahlung effect, which in turn creates photons. A photon loses its energy and changes direction by physical events such as photoelectric effect, coherent and incoherent scattering, and pair production (X-5 Monte Carlo Team, 2003). A positron is created during the pair production event. A positron experiences similar scattering events like electrons and annihilates with electrons. MCNP considers all the physical events for each particle by employing different types of cross sections. In this work, Nickel-63 is the beta emitter which has a maximum beta particle energy of 66.7 keV. Thus, the photon energy loss compared to the atomic excitation and ionization, which is the radiation yield, is on the order of 10^{-4}. MCNP uses the continuous slowing down approximation (CSDA) method to estimate the energy loss by collisional stopping power. It also uses Goudsmit-Saunderson's theory for the multiple scattering method to estimate the angular deflections of electrons using the numerically tabulated Riley cross section for electrons under 256 keV. The Moller cross-section is used in MCNP to calculate the generation of knock-on electrons.

Electrons are tracked down to 20 eV in this work. MCNP uses two different algorithms such as the condensed history and the single event method depending on the energy of a particle (Pelowitz, 2013; Hughes, 2012, 2013). The condensed history algorithm is applicable for the energy range of 1 keV to 100 GeV (Pelowitz, 2013), where it condenses multiple electron interactions in each logarithmic energy step size. It is computationally expensive for the electron transport to track all the interactions as it goes through a large number of collisions due to long range coulomb interactions for small energy loss (Hughes, 1996). Thus, the net effect of energy loss and angular deflection are estimated in the condensed history algorithm within a small energy step size. On the other hand, MCNP uses the single event method for particles with energy below 1 keV to 10 eV (Hughes, 2013). In the single event method, MCNP calculates the path lengths for all four physical events such as elastic scattering, atomic excitation, knock-on, and bremsstrahlung, then, takes the shortest path length of the associated physical events. It estimates the energy loss and angular deflection from the cross sections of the selected physical events. The average behavior of the physical system such as the energy deposition was inferred by MCNP from the statistics of individual particles.

3. Precise beta spectrum vs generalized beta spectrum for MCNP input

The amount of energy deposited and the depth of penetration of the beta particles emitted by the radioisotope source depends on their initial kinetic energy. Examples of radioisotopes that undergo radioactive decay by emitting beta particles are Ni-63, Sr-90, S-35, and P-32 (Alam and Pierson, 2016). Each beta particle emitted in decay has a continuous energy spectrum between zero and a maximum value. This maximum beta particle energy varies for different radioisotopes. The result is that each radioisotope will have a continuous energy