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Prediction of betavoltaic battery output parameters based on SEM measurements and Monte Carlo simulation

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HIGHLIGHTS

- New procedure for betavoltaic battery output parameters prediction is described.
- A depth dependence of beta particle energy deposition for Si and SiC is calculated.
- Electron trajectories are assumed isotropic and uniformly started under simulation.

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ABSTRACT

An approach for a prediction of ^{63}Ni-based betavoltaic battery output parameters is described. It consists of multilayer Monte Carlo simulation to obtain the depth dependence of excess carrier generation rate inside the semiconductor converter, a determination of collection probability based on the electron beam induced current measurements, a calculation of current induced in the semiconductor converter by beta-radiation, and SEM measurements of output parameters using the calculated induced current value. Such approach allows to predict the betavoltaic battery parameters and optimize the converter design for any real semiconductor structure and any thickness and specific activity of beta-radiation source.

1. Introduction

Miniature nuclear batteries become increasingly attractive as the long-life energy source for many applications, in particular, for powering microelectronic and microelectromechanical devices. A promising technique for radioactive decay energy conversion into electric current is based on the direct conversion of beta particle energy by semiconductor Schottky barriers or p-n junctions, which are the key part of a betavoltaic battery. ^{63}Ni is one of the most suitable radioisotope source for such application because of its pure beta particle emission, long half-life about 100 years and relatively low beta particle energy that allows to minimize a radiation damage of semiconductor convertor. Though numerous betavoltaic microbatteries have been experimentally investigated and demonstrated (see references in Zuo et al., 2013; Gui et al., 2016), their efficiency is much lower than that predicted theoretically. That could mean that the battery design is not optimal and/or that theoretical predictions are unreliable. In the same time, improving the conversion efficiency is very important in betavoltaic design because of the high cost of materials and manufacturing, and limits on the volume or weight of a device.

In the most cases for a simulation of beta element performance the Monte Carlo technique is used to calculate the energy deposition and expressions known from the physics of semiconductor devices or device simulators are used to calculate the output parameters of batteries. However, in many theoretical papers beta particles interaction with electrons and nuclei inside the ^{63}Ni source was neglected (San et al., 2013; Liu et al., 2014) although it essentially affects the beta particle energy spectrum, total number of emitted particles and their angle distribution. Sometimes, the average energy of beta particles emitted from the ^{63}Ni nucleus rather than the correct beta energy spectrum is used to simulate the battery performance (Wu et al., 2011; Yao et al., 2012; Munson et al., 2015). Calculations of betavoltaic battery output parameters without real semiconductor converter characterization allow to predict some limiting values but not the real parameters for a particular structure. All these approximations can be reasons for unreliable predictions. Thus, it can be stated that an accurate simulation model to guide the design of betavoltaic

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batteries is lacking up to now that could become an obstacle for their further development.

Since a fabrication of a highly enriched isotope material is very expensive and the technology of its deposition is insufficiently developed, to optimize the semiconductor converters and to estimate their effectiveness an imitation of beta-radiation source by e-beam of scanning electron microscope (SEM) can be used (Chandrashekhar et al., 2006; Tin and Lal, 2009; Ulmen et al., 2009; Pavlov et al., 2013; Zaitsev et al., 2014). When SEM is used for an imitation of beta-radiation a question about the appropriate beam energy and current arises. In many cases beam energy of 17.4 keV, corresponding to the mean energy of beta particles emitted from ^{63}Ni, was chosen for such purpose. However, as shown by Zuo et al. (2013), for a finite thickness of ^{63}Ni source the energy spectrum of beta particles changes significantly due to elastic and inelastic scattering and absorption. Moreover, as shown by Polikarpov and Yakimov (2016), the depth distribution of excess carrier generation rate under the beta radiation is qualitatively different from that for any monoenergetic electron beam. Therefore, it is impossible to imitate the beta radiation with a SEM e-beam by a corresponding choice of one or a few beam energies and other approaches should be developed for such imitation.

An approach for the adequate SEM imitation of beta emission for semiconductor converter characterization is discussed in the present paper. The approach to the problem consists of three parts: (1) a Monte Carlo simulation that predicts the depth dependence of excess carrier generation rate inside the semiconductor converter, (2) a determination of collection probability based on the electron beam induced current (EBIC) measurements and a calculation of induced current, and, (3) SEM measurements of output parameters using the calculated induced current value.

2. Short circuit current calculation

As mentioned above, it is impossible to imitate the beta-radiation with a monoenergetic electron beam. Therefore our strategy of using SEM as a beta-radiation imitator consists in a calculation of short circuit current induced by beta particles using the depth dependence of excess carrier generated rate calculated by the Monte Carlo technique and the collection probability obtained from the EBIC measurements on the structures playing a role of energy converter. This approach is based on the work of Donolato (1985), who showed that for a planar structure the collected current can be calculated as

$$I_c = \int_0^d h(z)\psi(z)\mathrm{d}z, \tag{1}$$

where z is the depth (the distance from the irradiated surface), $h(z)$ is the depth dependence of the electron-hole (e-h) pair generation rate proportional to the energy deposition distribution, $\psi(z)$ is the collection probability, i.e. the probability that a minority carrier generated at a depth z below the surface will reach the depletion region, d is the structure thickness. It should be stressed that the collection probability is a function of device design and semiconductor parameters only while the e-h pair generation rate is determined by the primary electron energy, incident angle and the material of semiconductor converter.

3. Monte-Carlo simulation of electron-hole pair generation rate

A beta particle is essentially electron that is emitted from the nucleus. The particle transport in a medium is a random process due to numerical elastic and inelastic collisions, following a statistical rule based on the movement status of all particles. In the most cases for a simulation of this process the Monte Carlo technique is used. Beta particle interaction with a semiconductor material is only considered in many theoretical papers concerning betavoltaic battery performance, and beta particle interaction with electrons and nuclei inside the ^{63}Ni source is neglected (San et al., 2013; Liu et al., 2014). However, this interaction essentially affects the beta particle energy spectrum, total number of emitted particles and their angle distribution. Sometimes, the average energy of beta particles emitted from the ^{63}Ni nucleus rather than the correct beta energy spectrum is used to simulate the battery performance (Wu et al., 2011; Yao et al., 2012; Munson et al., 2015) that can results in an unreliable prediction.

In the present work the home-made Monte Carlo program was used (Pavlov et al., 2013; Zaitsev et al., 2014). The calculation algorithm was specially adapted for the fast simulation of multilayer structures. The structure simulated consists of two principal layers: a thick semiconductor structure and the radioisotope Ni layer (the beta particle source), whose thickness can be varied. In turn, the semiconductor structure may consist of one or a few layers, i.e. it may include upper metallization and/or passivation layers. For the description of electron–electron collisions, the approximation of continuous energy losses was applied, and for elastic collisions of electrons with nuclei the screened Rutherford scattering cross-section was used (Reimer, 1998). The electron trajectories were assumed to start uniformly over the radioisotope layer thickness and isotropically along the electron emission direction. For the initial electron energy the spectrum of beta particles for ^{63}Ni (Preiss et al., 1957) was used. The specific activity was used as a parameter that allows to simulate betavoltaic element for the sources with a real ^{63}Ni content. Moreover, such model takes into account self-consistently the backscattering from a semiconductor convertor and its dependence on incident angle (Polikarpov and Yakimov, 2013). It should be stressed that such simulation allows to calculate directly the energy losses in the depth of the semiconductor for any source thickness and specific activity. The e-h pair generation rate dependence on a depth is obtained from the energy losses using the average energy E_i necessary for the e-h pair creation. As shown by Kobayashi (1972) E_i can be estimated as $E_i = 2.59 \cdot E_g + 0.71$ eV, where E_g is the semiconductor bandgap.

As an example, the generation rate dependences on a depth in 4H-SiC calculated for a few thicknesses of radioactive source with 15% of ^{63}Ni are presented in Fig. 1. It is seen that at a large enough depth these dependences can be described by the exponential

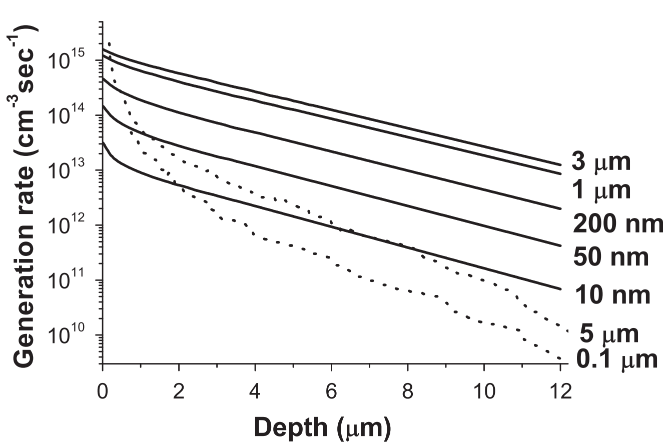

Fig. 1. Depth distributions of excess carrier generation rate $h(z)$ calculated for beta particle Ni source with an activity of 10 Ci/g and thicknesses of 10, 50, 200, 1000 and 3000 nm. Curves from Fig. 3 (Gui et al., 2016) for 100 and 5000 nm are shown by dotted lines for a comparison.