Monte Carlo simulations of electron trajectories for the study of betavoltaic battery configurations

E Napchan, J Benarroch

DLM Enterprises, London NW6 1QH,
eli@napchan.com

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With increase in demand for portable power the goal of battery development is to produce small, light, safe, high power and very long lasting batteries. Betavoltaics batteries use semiconductors to convert beta particles (electrons) emitted from a radioactive source, much like photovoltaic panels convert sunlight to electricity. A significant difference between both technologies is that the source can be within the devices themselves for betavoltaic cells, while the radiant sun energy comes from outside the outside for photovoltaic devices. A further difference is that betavoltaic cells can be stacked up. An example of a conceptual suggested betavoltaic battery, comparable to an AA battery, consists of 20 layers of betavoltaic diodes, each of which is approximately 42 µm thick, with Promethium being the nuclear material used. Promethium (Pm-147), with a half-life of 2.62 years, was used in the first batteries for pacemaker devices, but these were replaced by cheaper lithium-ion batteries with approximately 10 years life (see historical review by L. Olsen in [1]).

The simplest structure for a betavoltaic battery consists of the beta layer on top of a semiconducting junction in which the electrons produce electron-hole pairs, which are collected at contacts on both sides of the junction. Beta emission in the layer is considered isotropic within the layer, with randomization of the emission location and the emission characteristics. Each electron emission is isotropic in a sphere, calculated using the evaluation of direction cosines as given by [2]. The energy of the emitted particle is calculated based on the nuclear properties of the material, and the emission location is randomized within the radioactive layer.

The Monte Carlo simulation program used is called MC–SET and is derived from the work by D. C. Joy in [3], modified to include energy calculations and deal with multi-layers, among other changes. A version of the simulation is available on-line, see [4], along with additional information about the methods used. The simulation is designed for electron microscopy, and in particular SEM conditions, and for studying the beam energy deposition process in the sample under observation. For this work the simulation was modified from the case where the starting position, direction and energy of the incident electron was constant for all electrons, as in the case of an electron beam in the SEM, to the case where the location, energy and direction of emission is calculated based on random distributions, as applicable to beta emission from a layer. The simulation tracks each electron in its trajectory inside the specimen, and at each step calculates locally the energy lost by the electron. The energy deposited from all the electrons in the simulation is stored in a finite 3-dimensional energy matrix. Other parts of the electrons energy, such as backscattered, transmitted and out to the device electrons is also recorded during the simulation. This energy matrix consists of $N \times N \times N$ elements, where N can be changed depending on device dimensions. A further parameter that is setup for each simulation is the size of the energy matrix (llz), which affects the simulation resolution.

The simulated device consists of layers which can be of two types: spherical or slabs, the later only used for the current simulations. The physical material parameters used for the layers in the simulation include the atomic number and mass, and the density.

The purpose of this investigation is to describe a methodology for simulating beta voltaic batteries, with different geometric configurations. A standard combination of materials is used, and the relationship between the nuclear radiation emission and the energy obtainable is evaluated. This is done by calculating electron trajectories in the device, and from these the energy deposited at different locations (depths).

Figure 1 presents the depth dose (energy at depth) for electron beam penetration into a bulk Ni specimen, with the beam direction normal to the surface. The two selected energies correspond to the average beta emission energy and the maximum beta energy for the Ni-63 isotope. The high energy depth dose indicates that absorption in the Ni layer occurs at depths of up to about 10 um, which gives an upper limit for the thickness on a Ni-63 layer. The other curve indicates that for the average energy, all electron energy is absorbed within 1 um of Ni-63. Figure 1 inset presents the depth dose for a layered structure of Si-Ni-63-Si, for 2 um Ni-63 thickness. This curve shows the relative amounts of energy deposited in the Ni-63 and the Si layers, the latter being the effective maximum energy available for conversion. Figure 2 gives the energy deposited in one of the Si layers, for increasing values of Ni-63 thickness. The left hand curve corresponds to same activity for all layers, i.e. same number of beta emissions, while the right hand curve corresponds to all layers having the same specific activity (beta emissions per gram), corresponding to a typical Ni-63 isotope specific activity of 15 Ci/gr.

[1] L Olsen review in City Labs Inc., FL 33030 USA, www.citylabs.net/content/BetavoltaicHistory.pdf
[2] Direction cosines for isotropic spherical emission taken from mathworld.wolfram.com/SpherePointPicking.html
[3] “Monte Carlo Modeling for Electron Microscopy and Microanalysis”, D. C. Joy, (Oxford University Press, 1995)
[4] MC–SET simulation program, web site http://www.mc-set.com

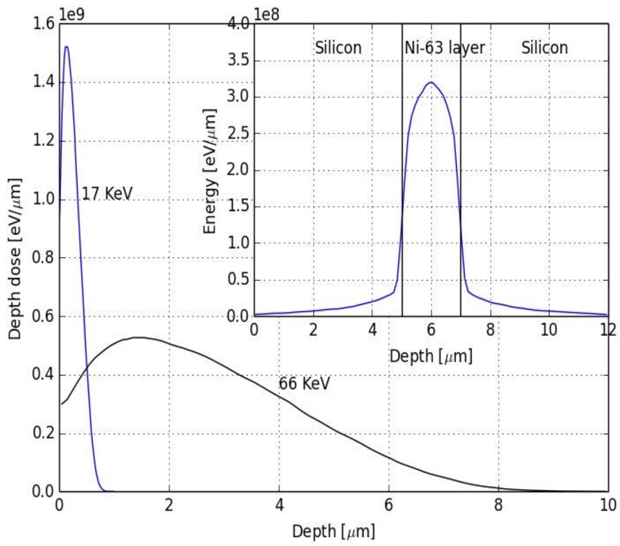

Figure 1. *Ni electron depth dose for 2 energies based on Ni-63 emission data and (inset) electron depth dose for Si-Ni-63-Si device*

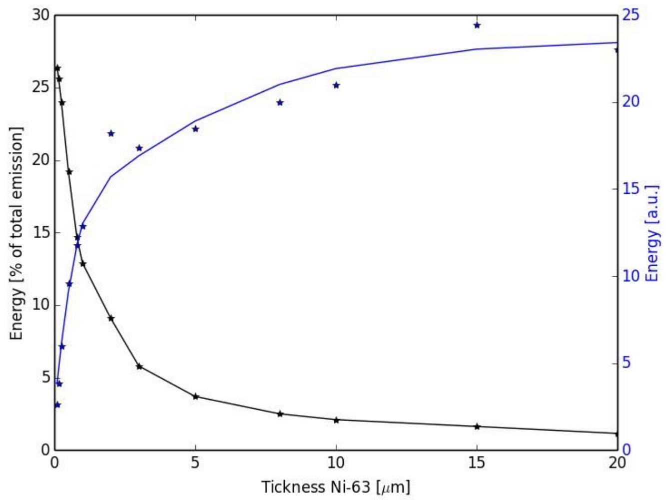

Figure 2. *Relative amount of beta energy emission from Ni-63 layer deposited in Si layer*