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GEANT4 simulation of implantation profiles for positrons injected in solids from radioactive sources ^{22}Na and $^{68}Ge/^{68}Ga$

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Abstract. We calculated theoretically the mass absorption coefficients for positrons emitted from the commonly used sources ^{22}Na and $^{68}Ge/^{68}Ga$ in numerous materials. For this purpose, we used the tool kit GEANT4 which allows to generate the implantation profile. An excellent agreement between the experimental profile and the calculated one was achieved. The calculated values of the mass absorption coefficients coincide well with the experimental values determined by the DSIP method.

Key words: positron annihilation • implantation profile • absorption coefficient • GEANT4 tool kit

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Introduction

The physics of positrons is an important discipline for science, industry and medicine. The fate of positrons injected into a solid material consists of several stages. After the implantation from a radioactive source positron loses its energy as a result of strong coupling with electrons and ions. It has only thermal energy and is in a thermodynamic balance with the environment at the end of an implantation stage. Then, the positron walks randomly with thermal energies in the sample and penetrates a volume occupied by ca. 10^9 atoms. Finally, annihilation and emission of two energetic photons of ca. 511 keV end its life.

It is a custom to describe the implanted positrons emitted from radioisotopes described by the exponential function of depth with only a simple parameter, i.e. linear absorption coefficient, noted as follows: α_+. This coefficient depends on the positron end-point energy and the material constants.

In many papers, the simple empirical formula of α_+ which was established over 58 years ago by Gleason *et al.* [4] is quoted. Theoretical calculations of the coefficient are difficult and attacked rarely. Recently, the computations by means of EGS4 codes have shown the possibility of such calculations [3]. In this paper we propose to use other codes, i.e. GEANT4 for theoretical calculations of this coefficient. It allows getting the implantation profiles and extract absorption coefficients α_+ for many materials. These calculations will be presented for positrons emitted from commonly used ^{22}Na and $^{68}Ge/^{68}Ga$ radioisotopes. A comparison with the recent experimental data will be performed.

The GEANT4 codes

GEANT4 (GEometry ANd Tracking) is a modern tool kit for simulations and visualizations phenomena in the field of high energy physics, atomic nucleus, elementary particles and technology [1]. It realizes Monte Carlo method, which allows tracing the scattering processes in a wide energy range. This tool kit makes it possible to define, vizualize and control bodies with complicated geometry, define centres and materials, easy selection of particles, energies and other layout properties. The standard electromagnetic processes are included in a set of data libraries. There are the essential processes like: photoelectric effect, Compton and Rayleigh scattering, bremsstrahlung and ionization, second electrons emission, the Auger effect and others. A good description for most processes is between 1 keV to 100 GeV. Obviously, some effects work correctly in a range of lower energies like bremsstrahlung which operates from 10 eV well and the Rayleigh and Compton scatterings which work even from 1 eV. For these reasons, we postulated that the GEANT4 is a suitable tool for simulation of positrons' transport's fate in a condensed matter.

The simulations procedure

In our calculations we used the following well-known formula [5] for energy spectrum of positrons emitted from both isotopes:

$$n(E, E_{max}, Z) = A\,F(E, -Z)(E_{max} - E)^2 \cdot (E+1)\sqrt{E(E+2)} \quad (1)$$

where

$$F(E, Z) = 2\pi\eta[1 - \exp(-2\eta)]^{-1} \quad (2)$$

and $\eta = \alpha Z/\beta$, α is the fine-structure constant, β is the relation of positron's speed to the speed of light, A is a normalization constant. End-point energy E_{max} for positrons emitted from a ^{22}Na source is equal to 0.545 MeV and 1.85 MeV for ^{68}Ge/^{68}Ga. The above spectrum served for obtaining the distribution function from the following formula:

$$D = \int_0^E n(E, E_{max}, Z)\,dE \quad (3)$$

Discreet values of this function were implanted in GEANT4 codes. The energy of emitted positron is determined using the following equation:

$$E = D^{-1}(x) \quad (4)$$

where x is a random number from 0 to 1 generated in the codes of GEANT4.

The positrons with such energies emitted from a point source randomly at a solid angle were traced in the material. The coordinates of annihilation spots were gathered and the histograms of depth were plotted and analyzed. In the simulations we assumed that the point source of emitted positrons is located between two 7 μm thick kapton foils, which correspond to the typical positron experiments. About one million positrons were traced to get proper results suitable for further analysis.

The positron implantation profiles

In our simulations we created the geometrical stack which was an exact copy of experimental configuration, i.e. isotope is enveloped in a kapton foil of 7 μm thick which is embedded in two identical samples. In Fig. 1 the simulated implantation profile for positrons emitted from the ^{22}Na source to Al is depicted. As it was reported in Ref. [3], the profile has the shape of a cup-like function. The number of positrons decreases along with the depth increase. There are two essential regions. In the first one, which is near the source, the curve falls rapidly. In the second one the curve has an exponential shape which can be described by the well-known formula:

$$N(z) = N_0 \exp(-\alpha_+ z) \quad (5)$$

where N_0 is a normalization constant, z is the depth of annihilation. The fit of Eq. (5) within this region allows obtaining the linear absorption coefficients α_+ (the black straight line in Fig. 1). The reciprocal value of the linear absorption coefficients called the mean depth of implantation in this case is equal to 89.6 μm.

For comparison, we performed the measurement of the implantation profile for Al using a DSIP (depth scanning of implantation profile) method [2]. In this method the sandwich composed of the radioactivity source between two identical samples is placed in front of the slit between two lead bricks. A coaxial detector is placed behind the slit. A micrometer screw allows shifting the samples in the direction perpendicular to the slit. In this way registration of different annihilation depth is possible. The gamma particles from annihilation at a given depth pass through the slit and are counted in the detector. This allows creating the positron implantation profile for a given material where positrons are injected.

In order to compare the simulated profile with experimental one we convoluted the simulated profile

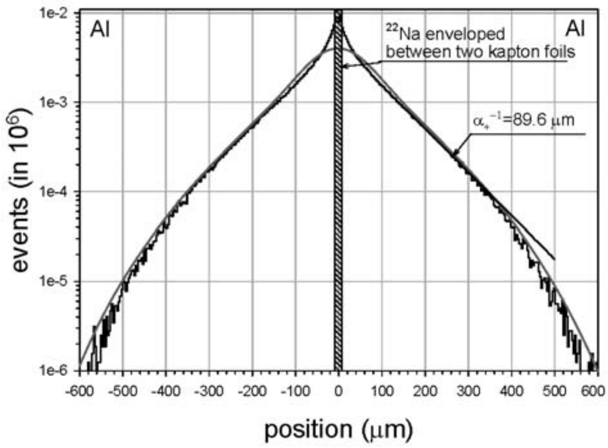

Fig. 1. The normalized implantation profile of ^{22}Na positrons in Al obtained from GEANT4 simulations. The grey line is the convolution of Gaussian function which represents the resolution function in the experiment. The straight line is the least-squares fit of exponential region.

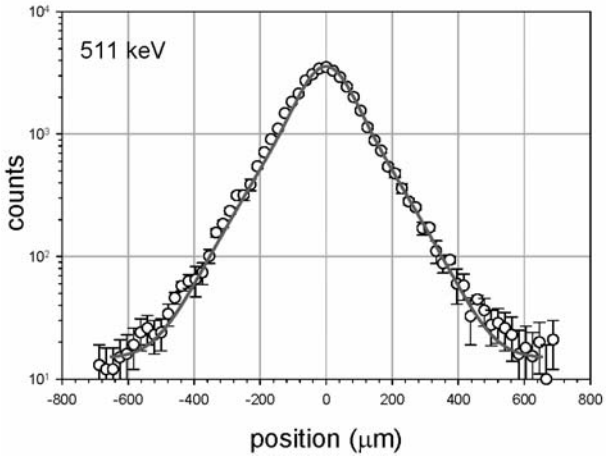

Fig. 2. The comparison of implantation profiles for positrons emitted from ^{22}Na to Al obtained by means of experimental DSIP method (open circles) and generated by GEANT4 taken from Fig. 1, grey line, after adding a constant value which represents the background.

with the typical resolution of the apparatus and added a constant value representing a background always present in the experiment. The convolution of Gaussian function with the resolution of slit FWHM = 120 μm for GEANT4 profile for Al was done (see the grey line in Fig. 1). Figure 2 shows both the simulated and the experimental profiles. This convinces us that the simulated procedure works well. Then, the simulations for other selected materials were performed in order to extract the linear absorption coefficient similar to the above for Al. The results, i.e. the mass absorption coefficient: α_+/ρ where ρ is the material density, are depicted in Fig. 3 as a function of atomic number.

In this figure the values from the GEANT4 simulation (grey circles) and experiment (closed circles) are presented. The experimental data were taken from Ref. [3] and were measured using the DSIP method. Once again the dependency of the mass absorption coefficient on the atomic number was confirmed. Additionally, the perfect agreement between the theoretical and experimental values was achieved. The solid lines are the best fits of the power function to the points received from the GEANT4 simulations. The following dependencies are obtained:

$$\alpha_+/\rho\ [\mathrm{cm^2/g}] = (29.3 \pm 1.4) Z^{0.15 \pm 0.01} \tag{6}$$

for ^{22}Na and

$$\alpha_+/\rho\ [\mathrm{cm^2/g}] = (3.73 \pm 1) Z^{0.23 \pm 0.01} \tag{7}$$

for $^{68}Ge/^{68}Ga$. These equations are in good agreement with the formula calculated for experimental points [3]. The deviations are within the accuracy. This follows the dependency of the mass absorption coefficient on the atomic number detected experimentally.

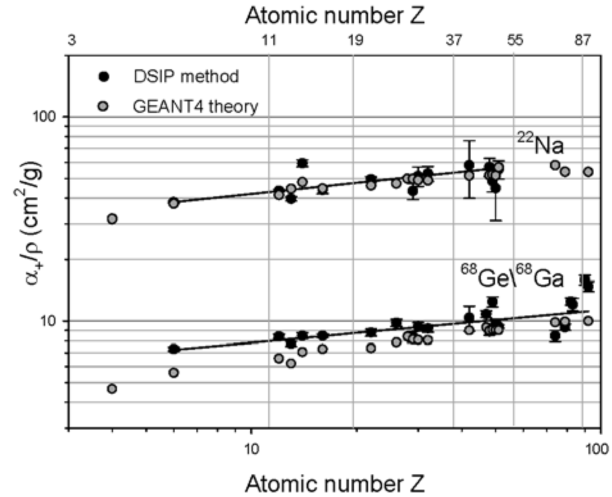

Fig. 3. The values of the mass absorption coefficient as the function of atomic number Z for positron from ^{22}Na and $^{68}Ge/^{68}Ga$ sources. The closed circles derive from the experiment [3]. The grey circles represent the results from GEANT4 simulations. The solid line is the best fit of the power function to the calculated points.

Conclusions

The GEANT4 turned out to be a good tool kit for the simulations of the positron transport in the matter. The implantation profiles, determined using this tool kit, allow us to obtain the profile which fitted well with the experimental values obtained by the DSIP method. The mass absorption coefficients generated by the simulations which are in good agreement with the experimental values prove that GEANT4 can be used in the field of positron physics successfully.

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