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Design and Implementation of Alpha Energy Spectrum Simulation Software for the PIPS-Geant4 Model

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Abstract

In order to further develop the optimization technique of α-particle energy spectrum detection parameters based on Monte Carlo simulation method, this paper uses PyQt5 to design a software that calls the Monte Carlo simulation package Geant4 for α-particle energy spectrum simulation research. The physical model of PIPS(Passivated Implanted Planar Silicon) detector for α-particle measurement is established, and the simulated physical processes, model materials, and parameters such as geometry and composition of the particle source are corrected according to the actual α-particle measurement conditions, and the functions of modifying the parameters of the particle source and detector are visualized by combining with the PyQt5 interface development platform. Visualization. The simulation experiments are carried out under multiple probe distances and different vacuum pressures, and the acquired energy is deposited into a spectrum and then broadened by the EMG (Exponentially Modified Gaussian) response function model. The results show that the EMG response function model broadening effect is good. The results of this paper verify the reliability of the Geant4 simulation software in the study of α-particle energy spectrum, which can intuitively modify the measurement conditions of α-particle energy spectrum, simplify the simulation steps, improve the simulation efficiency, and provide a powerful tool for the optimization of the detection parameters of α-particle energy spectrum based on Monte Carlo simulation method.

Keywords

PyQt5; Geant4; PIPS; Response Functions.

1. Introduction

α-particle energy spectroscopy is an important method of α-nuclide measurement, different thickness, area, angle and vacuum and other complex sample conditions have a greater impact on the α-particle energy spectroscopy measurement, therefore, to explore the different measurement conditions and sample types of α-particle energy spectroscopy analysis of the influence of the law has become an important basis for improving the accuracy of quantitative analysis of α-nuclides, the traditional experimental-based research method of the measurement of the sample usually need to be chemically separated before the measurement of the time-consuming and high cost[1,2]. With the development of computer technology and the wide application of numerical simulation technology, the optimization of α-particle energy spectrum detection parameters based on Monte Carlo simulation methods has become an important and convenient means for the study of α-particle energy spectrometry measurement technology, which can effectively simulate a variety of measurement conditions and

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sample types[3]. Among them, Geant4 is a Monte Carlo simulation package commonly used in particle simulation technology, which provides a variety of particles, geometric description classes of models and a series of visualization interfaces and other tools, and has the advantages of multi-physics process simulation capability, flexible geometric models, open source code, rich toolbox and so on[4].

This work is based on Geant4 to simulate the α-particle energy spectrum and to develop a user-friendly software for simulation and data visualization. The software is used to call Geant4 to accurately model the geometry of the virtual detector chamber, the simulated physical process and the shape of the radioactive source according to the actual detector parameters, and to simulate the α-particle energy spectrum under different conditions of vacuum level and source distance, to verify the feasibility of this Geant4 simulation software for the study of α-particle energy spectrum using the EMG response function model broadening. The obtained energy deposition spectrum is broadened using the EMG response function model, which verifies the feasibility of the Geant4 simulation software in the study of α-particle energy spectra, and provides a new method for the optimization of α-particle energy spectra detection parameters based on Monte Carlo simulation method.

2. The Theoretical Foundation

(1) Alpha Particle Measurement Influences

The factors affecting α-particle measurement mainly include physical processes and air pressure. Physical processes refer to the interaction process of α-particles in matter, such as scattering, ionization, etc. Different physical processes affect the characteristics of α-particles, such as transmission and energy deposition; changes in the air pressure will lead to changes in the energy deposition of incident particles in the detector, which affects the range of the incident particles in the air and the behavior of the transmission of incident particles in the detector, such as particle diffusion, drift, etc.

The electromagnetic physical processes interacting with α-particles in Geant4 can be realized by calling G4EmStandardPhysics(), which includes the processes of many kinds of charged particles interacting with matter, such as electrons and positrons, and takes into account many kinds of physical effects, such as ionization, excitation, and scattering, etc.; for the α-particles' decay process, it can be realized by using the G4RadioactiveDecayPhysics() and G4DecayPhysics() physical process models are implemented. For the relationship between air density and pressure, Geant4 can return the density of air through the function GetDensity() in the G4Material class[5]. For the relationship between air density and pressure, Geant4 can return the density of the material in g/cm3 through the function GetDensity() in the G4Material class, and get the pressure of the material through the GetPressure() function in the G4Material class[6]. When the air pressure changes, the atmospheric density will also change, air density and atmospheric pressure of the relationship between the formula shown in equation(1):

$$\rho = P * M / (R * T) \tag{1}$$

(2) Spectral Spreading

The energy deposition obtained from statistical Geant4 simulations, in the deconvolution of the α-particle energy spectrum, it is necessary to use the detector response function to describe the distribution of the energy peaks in order to fit the experimentally measured spectral data, in which the EMG response function model is able to more accurately analyze the α-energy spectrum consistent with the effect severity[7], and therefore it is used for α-simulated energy spectrum broadening. This response function model is shown in equation (2):

$$f(x) = \sum_{i=1}^{n} A_i \left[\frac{\eta_1}{2\tau_1} exp(1) erfc(1) + \frac{\eta_2}{2\tau_2} exp(2) erfc(2) + \frac{\eta_3}{2\tau_3} exp(3) erfc(3) \right] \tag{2}$$

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3. Experimental Design and Software Development

The steps of the overall research program of this paper are as follows:

① Build Monte Carlo model: according to the geometric structure and material composition parameters of the PIPS detector chamber, use Geant4's geometry module and physical material module to build a virtual PIPS chamber geometry model, particle source module to define the particle source and set up the simulation physical process.

② Simulation software design: use PyQt5 design software to call Geant4 to build the above PIPS chamber model and carry out simulation experiments, to realize the automatic control of Geant4 particle simulation.

③ Setting simulation conditions: simulate the α-energy spectra of the ^{238}Pu standard source at 500.0 Pa pressure for five different probe distances, and simulate the α-energy spectra of the ^{238}Pu standard source at 6.8 mm probe distance for four different air pressures.

④ Data analysis: the energy deposition spectra were broadened using the response function method, and the broadening effect was analyzed.

(1) Parameters of experimental apparatus

The detector used in the experiment is the ULTRA-AS series deep ion-implanted silicon detector (PIPS) of ORTEC, which has the advantages of high sensitivity and high resolution compared with the traditional α-energy spectroscopy detector, with an area of 600 mm², a radius of 13.82 mm, a dead layer thickness of 5 nm, and an effective thickness of the sensitivity layer of 350 μm, and the used ^{238}Pu standard surface source with an The effective radius of the ^{238}Pu standard surface source used is 10mm[8], Fig. 1 shows the physical diagram of the chamber of the PIPS-α spectrometer, and the overall materials used are shown in Table 1.

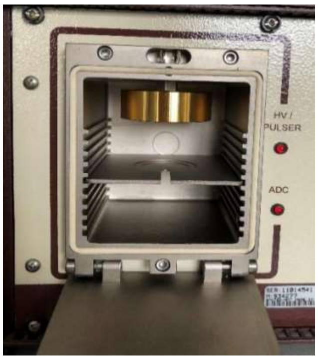

Fig. 1 Photo of PIPS-α spectrometer chamber

Table 1. PIPS detector chamber components, dimensions and materials

Part	Materials	Density(g/cm^3)	Size(mm)		
			inner radius	outer radius	half height
Probe top	Stainless steel	8.06	0	8	3.655
Probe	Stainless steel	8.06	0	13.82	6.175
Tray	Aluminum	2.7	34	25.82	1
Sample tray	Stainless steel	8.06	0	12	0.25
Slot stick	Aluminum	2.7	34	1.15	1
Dead layer	Silicon	2.33	0	13.82	2.5×10^{-6}
Silicon layer	Silicon	2.33	0	13.82	0.175
Rubber layer	Rubber	0.92	0	13.82	0.25
Brass layer	Brass	8.5	0	13.82	0.5
Polyethylene layer	Polyethylene	0.94	0	13.82	2

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(2) Geant4 Modeling

Geant4 was used to create a physical model of the PIPS detector chamber based on the aforementioned spectrometer-related parameters provided by ORTEC. A representative PIPS detector chamber model is shown in Fig. 2.

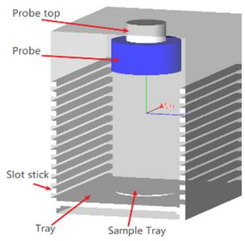

Fig.2 The physical model of PIPS detector

(3) Geant4 simulation software development

In order to solve the problems of the above Geant4 model experiment operation process is not intuitive, and can not directly modify the experimental parameters, the use of PyQt5 to develop a α-particle simulation software, to achieve the detector, the particle source information of the visualization of the editing and simulation experiments can be operated interactively[9]. Fig. 3 shows the functional block diagram of the software, and the Geant4 simulation module and the energy spectrum data analysis module are designed to realize the functions of inputting, editing and saving experimental parameters through interface controls.

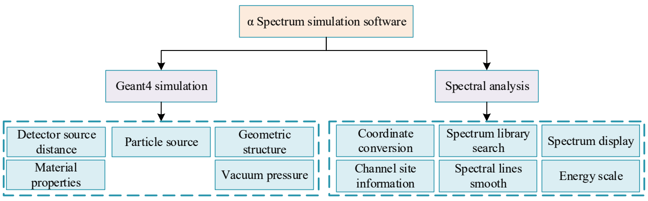

Fig.3 Block diagram of the overall software function

The technical route of the software to call Geant4 simulated particles is shown in Fig. 4. In PyQt5, different interface components interact and transfer data through the signal and slot mechanism, which can realize data transfer between multiple classes, making the software powerful interactive and scalable. Set the detector conditions and particle source type and number to be simulated, generate the detectorconstruction.cc file and the mac file respectively, call the shell command make to reconstruct the PIPS detector chamber model through subprocess.run(), call the executable file to run the particle source information of the mac file, and deposit the energy The energy deposition is saved as a csv file, and the energy deposition is spectroscopically generated using the logarithmic energy interval method[10], which is suitable for particles in a wide energy range and more accurately reflects the energy deposition in different energy ranges, and finally the response function is used to broaden and analyze the experimental and simulated spectral data.

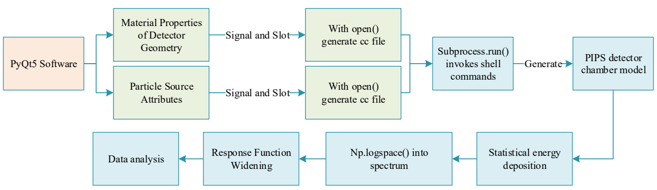

Fig.4 Simulation Software Technology Line

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In the main page, it contains the entrances of each function, energy spectrum data plotting, coordinate conversion and road site information, etc. Fig. 5 shows the main page of the software.

Fig.5 Software main page

The software realizes center of gravity smoothing, least squares smoothing and exponentially modified derivative smoothing EMD (Exponentially Modified Derivative Smoothing), and the scale method contains two kinds of linear and nonlinear scales, and the interface is as shown in Fig. 6, and the Monte Carlo simulation interface can be used to conveniently modify the attributes of the detector, the vacuum pressure, and the attributes of the radioactive source, and, moreover, it can be used to open an XML file to show the magnitude of energy share of multiple nuclides, as shown in Fig. 7.

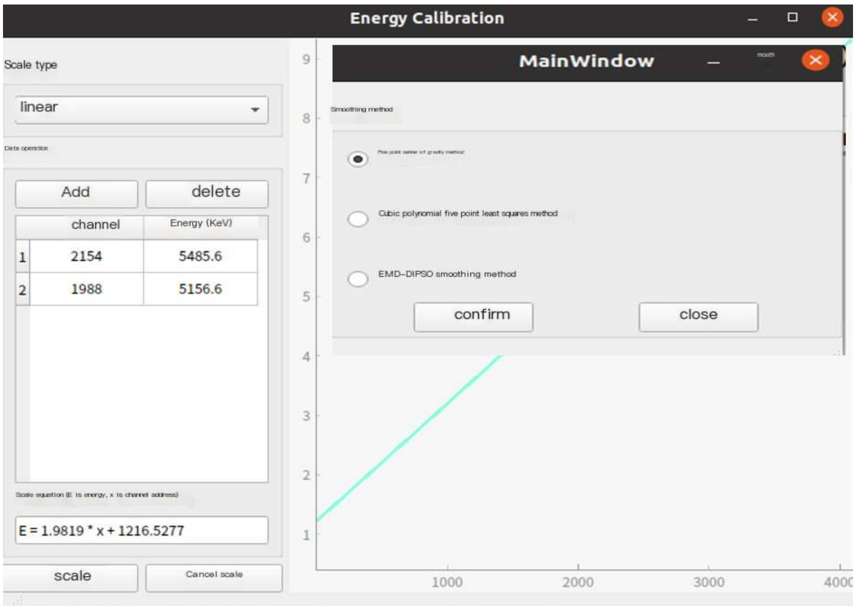

Fig.6 Spectrum Analysis

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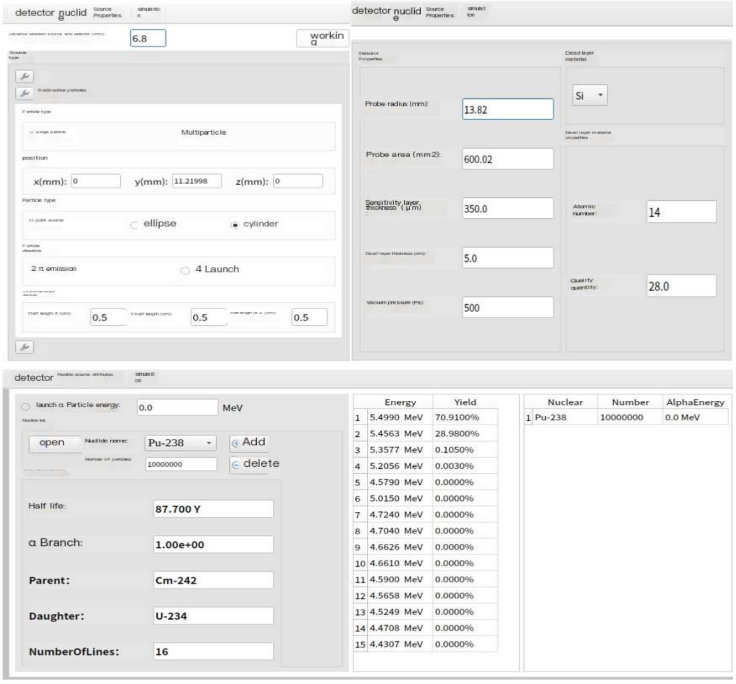

Fig.7 Monte Carlo simulation interface

4. Analysis and Discussion of Results

(1) Simulated spectral data broadening analysis

Using the software in this paper to carry out α-particle simulation experiments, the obtained energy deposition spectra are broadened using the response function method, in order to highlight the key points, only the data near the effective peak are shown for comparison, and the experimental results show that the broadened omnipotent peaks have good effects, and the red solid line in Fig. 8 and Fig. 9 indicates that the simulation of the un-broadened peaks of ^{238}Pu and ^{239}Pu is simulated in the form of the surface source at the distance of 6.8 mm from the probe under the vacuum pressure of 500 Pa. The black solid line shows the data after the response function broadening process.

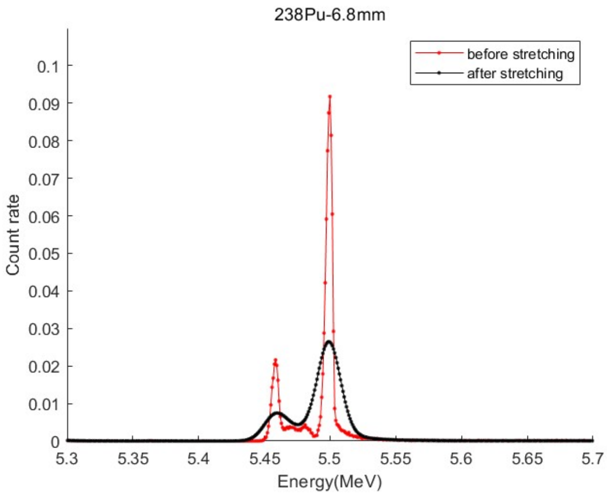

Fig.8 ^{238}Pu post-broadening

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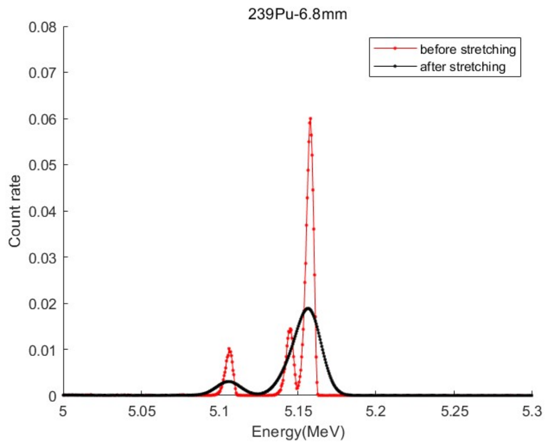

Fig.9 ^{239}Pu post-broadening

5. Conclusion

In order to further develop the optimization technique of α-particle energy spectrum detection parameters based on Monte Carlo simulation method, this paper is based on the Monte Carlo program Geant4, which accurately models the geometrical structure and physical process of the PIPS semiconductor Si detector, and adopts PyQt5 as the GUI programming library, to develop a software for visual editing the detector and particle source information and interactively manipulating the simulation experiments, and to broaden the obtained Energy is deposited into a spectrum and broadened using a response function, and the effect of the simulated spectrum broadening at different vacuum levels and the detection efficiency error between the simulated data and the experimental test data at multiple source distances are analyzed. The experimental comparison results show that the EMG response function model has good broadening effect, which verifies the feasibility of the Geant4 simulation software designed in this paper in the study of α-particle energy spectrum. At the same time, the software can not only be used to study the measurement of α-particle energy spectrum with different source distances and vacuum levels, but also to study the effects of α-particles with different types and sizes of radioactive sources on the distribution of energy deposition and the statistical error, with fast simulation speed and high accuracy, which provides practical tools for the optimization of α-particle energy spectra based on the optimization of the parameters of Monte Carlo simulation method, and also provides a useful path for the development of the related research, and it has a wide range of application value. wide range of application value.

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References

[1] Xu Yangyang, Tou Xianguo, Shi Rui, et al. Monte Carlo simulation of detection efficiency of PIPS-α spectrometer and its influencing factors[J]. High Power Laser and Particle Beams, 2017, 29(10): 155-160.

[2] Rui Shi, Xianguo Tuo, Jian Bo Yang, Yi Cheng, Honglong Zheng, Qibiao Wang, Chao Deng. A peak shape model with high-energy tailing for high-resolution alpha-particle spectra, European Physical Journal A, 2019, 55(8): 138-144.

[3] Liu Jiangping, Chen Qiang, Wang Zhixin, et al. Computational and Process Interface Software Development for 10MeV Industrial Irradiation Electron Accelerator GEANT4[J]. Journal of Radiation Research and Radiation Technology, 2022, 40(06): 62-69.

[4] Wei Tang, Jin-Gang Liang, Yi Ge,. et al. A method for neutron-induced gamma spectra decomposition analysis based on Geant4 simulation[J]. Nuclear Science and Techniques, 2022, 33(12): 38-50.

ISSN: 2414-1895 DOI: 10.6919/ICJE.202402_10(2).0001

[5] Díaz-Francés J A, Cortés-Giraldo M A, Jiménez-Ramos M C, et al. Simulation of the response of a PIPS detector using GEANT4 code[J]. Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2017, 875: 21-26.

[6] Moslehi A, Baradaran S, Taheri M. GEANT4 modeling of alpha particles detection efficiency for polycarbonate SSNTD[J]. Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2022, 1033: 166714.

[7] Pöllänen R. Performance of an in-situ alpha spectrometer[J]. Applied Radiation and Isotopes, 2016, 109: 193-197.

[8] Shi R, Tuo X, Cheng Y, et al. Applications of non-negative iterative deconvolution method in the analysis of alpha-particle spectra[J]. The European Physical Journal Plus, 2020, 135(2): 225.

[9] Tian Feng, Geng Changran, Tang Xiaobin, et al. Proton range monitoring based on picosecond detection using a Cherenkov radiation detector: A Monte Carlo study[J]. Applied Radiation and Isotopes, 2022, 180.

[10] Shao Jiang, Zhu Keyong, Liu Xiaochuan, et al. A general Monte Carlo method for polarized radiative transfer in multi-dimensional graded-index media[J]. Journal of Quantitative Spectroscopy and Radiative Transfer, 2022, 278.