CONCEPTUAL DESIGNING OF A SLOW POSITRON BEAM SYSTEM USING SIMION SIMULATION PROGRAM

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Abstract: The slow positron beam system is an important device in the study of positron physics and techniques, especially in materials research. Our report presents the obtained results in studying and applying a charged particles trajectory simulation program – Simion for building feasible design models for the system. Some positron beam trajectory calculation tests have been performed for comparison between the models. From that, a conceptual design model has been proposed as a basis for building a real slow positron beam system in the future in Vietnam.

Keywords: *Slow positron beam system, simulation program, Simion, conceptual design*

1. INTRODUCTION

Positron annihilation techniques play an important role in the study of micro-defect of materials, nanostructures, porous materials, surface analysis, etc. [1]. However, the study of surface structure, layers or interface regions cannot be performed with traditional isotope positron sources because the energy of the positrons emitted from the sources varies in a wide range (positrons from the isotope source with high energy go very deeply into the sample, which reduces the chance of positron interaction as well as the formation of positronium on the material surface) [2]. Slow positron beam systems have been developed to solve that problem. They are applied widely in materials science, physics of solid state, condensed matter and surface [2]. In general, the slow positron beam systems in the world have different designs but follow a general operating principle. A fraction of high energy positrons emitted from a radioactive source are slowed down (moderated) to become slow positrons with low energy of several eV. The positron beam is then pre-accelerated by a pre-accelerator and guided to an energy filter to separate the slow monoenergetic positrons out of the original beam. The separated slow monoenergetic beam is then guided through an accelerator to be accelerated to necessary high energy depending on research purposes, directed to the sample chamber and interacts with the investigated sample.

Center for Nuclear Techniques (CNT) has been using positron annihilation techniques including positron annihilation lifetime spectroscopy and Doppler broadening spectroscopy for studying some metal material properties, carbon nanotubes, and zeolite. However, the main positron sources used for these studies are ^{22}Na with continuous energy spectrum that limits the study of surface properties of materials. Therefore, the need to build a slow positron beam system at CNT in the future to perform such studies is essential. To ensure the construction feasibility of the system, necessary work in this early stage which needs to be done is to study and use an appropriate charged particles trajectory simulation program to conceptually design the system. We have used Simion as the main tool for the purpose of conceptual designing. Among typical simulation programs, Simion has been widely used to model ion optics problems including calculating and simulating electrostatic fields, magnetic fields and trajectories of charged particles flying through these fields. The program is highly interactive and has been used effectively in many research projects on designing and building slow positron beams at the Institute of Radiation Physics, Helmholtz-Centre Dresden-Rossendorf (Germany), Lawrence Livermore National Laboratory (USA), University of Bath (UK) and in other countries such as Romania, Israel, China [3-6]. Besides that, some initial simulation tests for the reference design of the SPONSOR system from the Institute of

Radiation Physics, Helmholtz-Zentrum Dresden-Rossendorf in Germany were performed successfully at CNT in 2017. The good agreement between our simulated results and experimental data from the SPONSOR system demonstrated that Simon can be used well for conceptual designing of a slow positron beam system [7].

This report presents results of applying Simion program to build some design models for the system based on design principles of some built systems in the world and propose a feasible conceptual design of the system that can be used to prepare for the stage of detailed engineering design and construction of the system in the future.

2. CONTENTS

2.1. Overview of Simion program

Simion is a software package used primarily to model electrostatic and magnetic fields and calculate trajectories of charged particles in these fields when introducing the electrode configuration with voltage and initial conditions of the particles [8]. Simion is intended to provide direct and highly interactive methods for simulating a wide variety of general ion optics problems such as modeling ion source and detector optics, ion traps, quadrupoles, etc. Electrostatic and magnetic fields can be modeled as boundary value problem solutions of a partial differential equation called the Laplace equation (or the Poisson equation). The specific method used within Simion to solve this equation is an over-relaxation technique, which is a finite difference method to obtain a best estimate of potentials for each point within the fields. After the electrostatic and magnetic fields have been obtained, a standard fourth-order Runge-Kutta method is used for numerical integration of the charged particle trajectory in three dimensions based on the particle definition parameters provided by users. In particular, Simion provides functions of extensive support in the definition of geometry, data logging, and visualization. One of the most useful features of Simion is the capability of using user programs inside the program. This feature allows users to directly utilize a variety of programming languages including Lua, C++, C, PRG, etc. to flexibly and efficiently extend simulation capabilities of the program.

2.2. Methods

According to several reference system designs, we have successfully built some simulation models that can be possible designs for the system by using Simion. Due to application limitations of the program, the design models are only used to simulate the operating principle of slow positron beam systems rather than specify detailed engineering designs. Three main individual simulation models of the slow positron beam system have been built including:

- The straight-shaped model using the ExB filter (figure 1)
- The 50^0 bent-shaped model based on the design of the SPONSOR system [9, 10] (figure 2)
- The 90^0 bent-shaped model based on the design of a slow positron beam system from Martin Luther University Halle-Wittenberg, Germany [11] (figure 3)

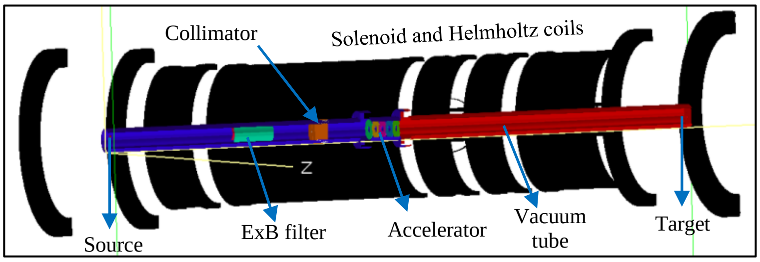


Fig 1. The straight-shaped model using ExB filter

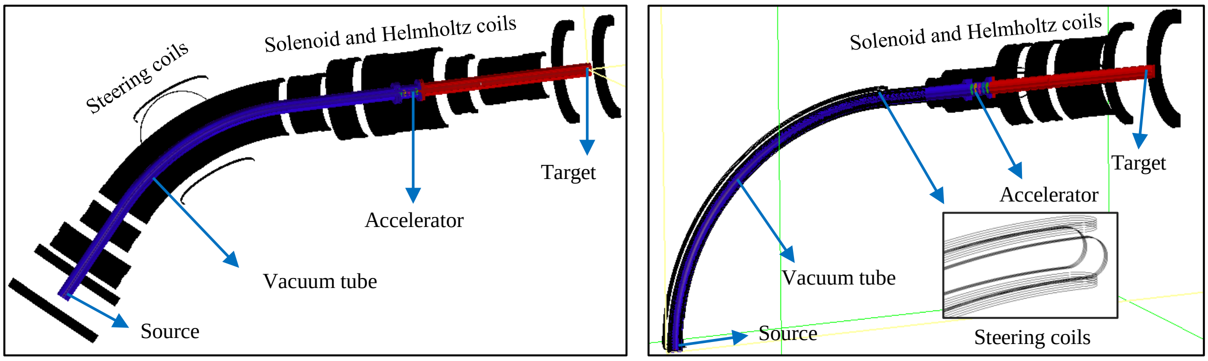


Fig 2. The 50^0 bent-shaped model (left) and the 90^0 bent-shaped model (right)

Some positron trajectory calculation tests have been performed for each model in order to investigate the influence of design parameters of each model on the quality of positron beam obtained on targets, thereby determining which model was the most reasonable design. The selected model has been proposed as a feasible conceptual design for the future system. Tables of design parameters for the proposed conceptual design include geometry parameters, electric parameters and design parameters of coils creating magnetic fields.

2.3. Results and Discussions

Case 1: Simulation of the trajectory of a monoenergetic positron beam

Simion has been used to calculate the trajectories for 1000 monoenergetic positrons in a beam emitted isotropically from a circular uniform distribution source with a radius of 2 mm for each model. The initial kinetic energy of the beam was 3 eV. The voltages that were applied to the pre-accelerator and the accelerator of each model were 27 V and 30 kV respectively. The simulation results are shown below in table 1, figure 3 and figure 4.

Table 1. The simulation results for trajectory of a monoenergetic positron beam

	Straight shaped model	**50^0 bent shaped model**	**90^0 bent shaped model**
Total number of positrons from source	1000	1000	1000
Total number of positrons coming to target	789	807	795
The ratio of positron number coming to target to total positron number	78,9%	80,7%	79,5%
Beam radius on target	**2,75 mm**	**2,39 mm**	**2,79 mm**

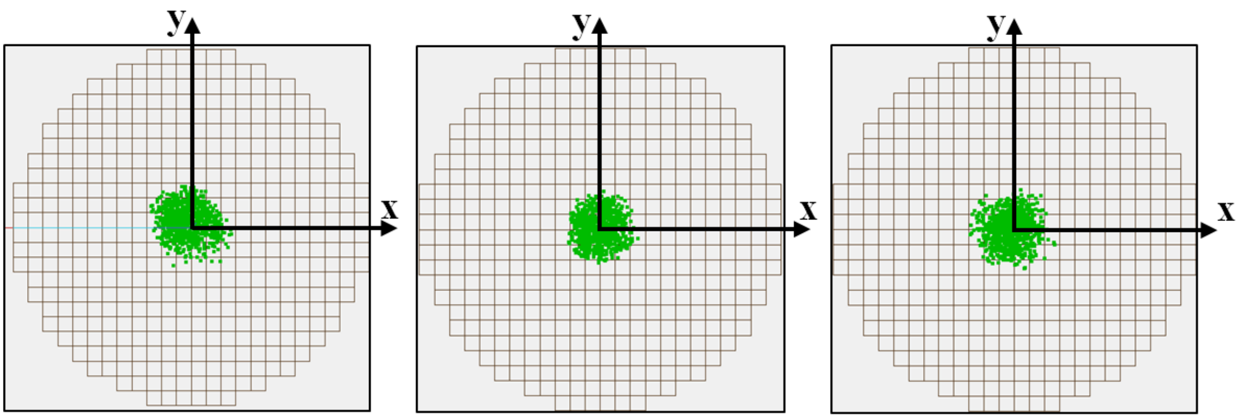
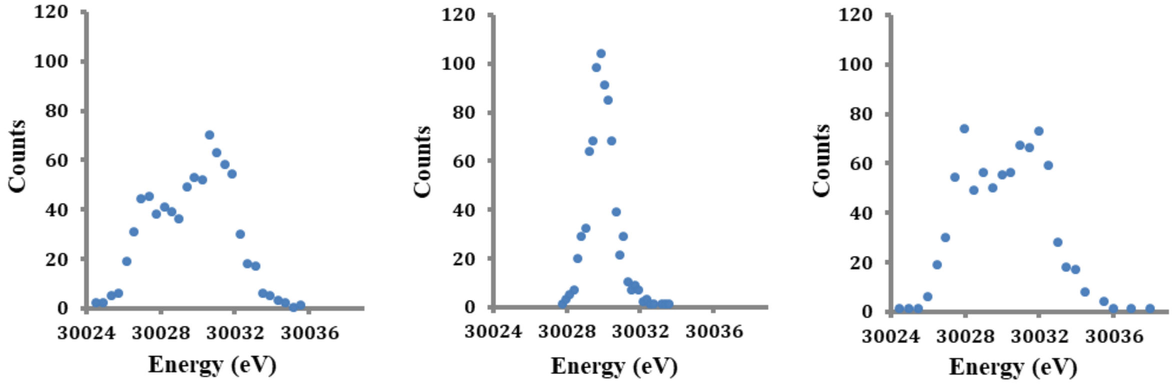


Fig.3. Distribution of positron beam on the target of the straight-shaped model (left), the 50^0 bent-shaped model (middle) and the 90^0 bent-shaped model (right)



(FWHM = 5.50 eV) **(FWHM = 1.34 eV)** **(FWHM = 5.71 eV)**

Fig.4. Energy distribution of positron beam on the target of the straight-shaped model (left), the 50^0 bent-shaped model (middle) and the 90^0 bent-shaped model (right)

From the results of the beam radius of the positron beam on the targets, it has been found that obtained positron beam in case of using the 50^0 bent-shaped model has better convergence compared to the other models. Furthermore, FWHM of the energy distribution of the positron beam on the target for the 50^0 bent-shaped model was smaller than those of the other models. It has shown that the obtained positron beam of the 50^0 bent-shaped model was more monoenergetic than those of the other models.

Case 2: Simulation of the trajectory of a monoenergetic positron beam in case that a solenoid deviated from its original position

Another trajectory calculation test has been done for each model with the same monoenergetic positron beam in case that the solenoid surrounding the accelerator of each model deviated from its original position. Distributions of positron beam on the target of each model have been investigated for comparison. We have simulated two situations that the solenoid deviations were 1 cm and 2 cm. The simulation results are shown below in figure 5, figure 6 and figure 7.

The comparison results below have shown that the solenoid deviation influenced the quality of the positron beam that comes to the targets. For the straight-shaped model, there were a few positrons obtained on the target in case of solenoid deviation of 1 cm. In the case of a solenoid deviation of 2 cm, we have even got no positrons coming to the target. For the 90^0 bent-shaped model, the obtained positron beam has deviated much more from the target center compared with that of the 50^0 bent-shaped model. The beam has even distorted its shape when increasing the solenoid deviation to 2 cm. Therefore, we have concluded that the 50^0 bent-shaped model in this simulation case would be the optimal model compared with the other models.

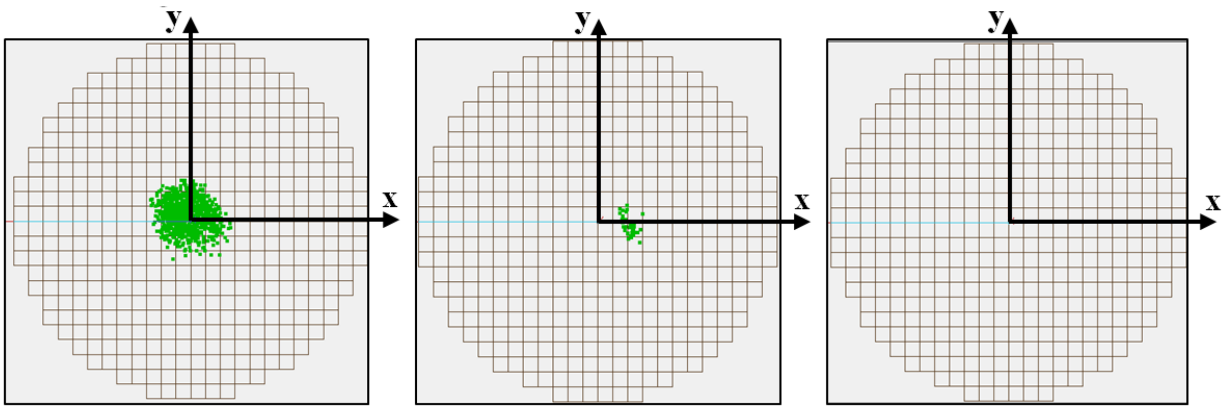


Fig.5. Distribution of positron beam on the target of the straight-shaped model in case of solenoid deviation of 0 cm (left), 1 cm (middle) and 2 cm (right)

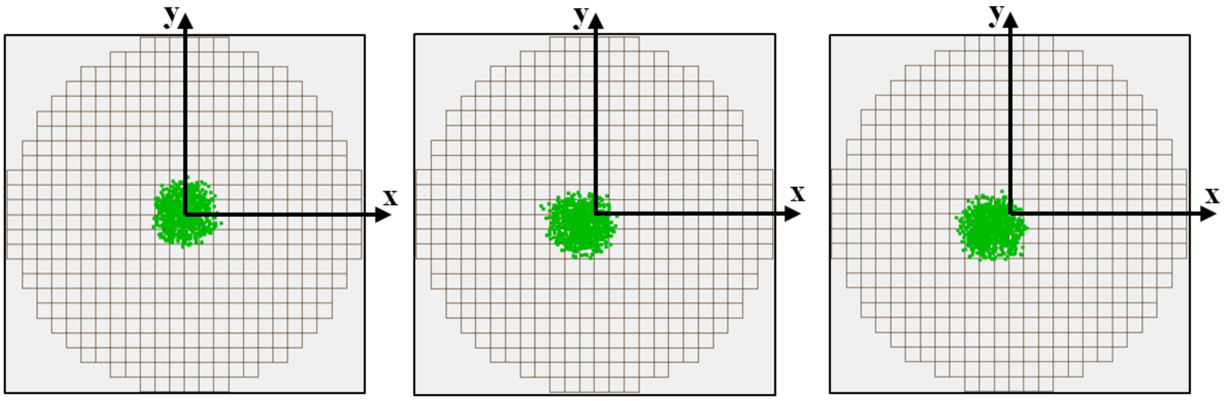


Fig.6. Distribution of positron beam on the target of the 50^0 bent-shaped model in case of solenoid deviation of 0 cm (left), 1 cm (middle) and 2 cm (right)

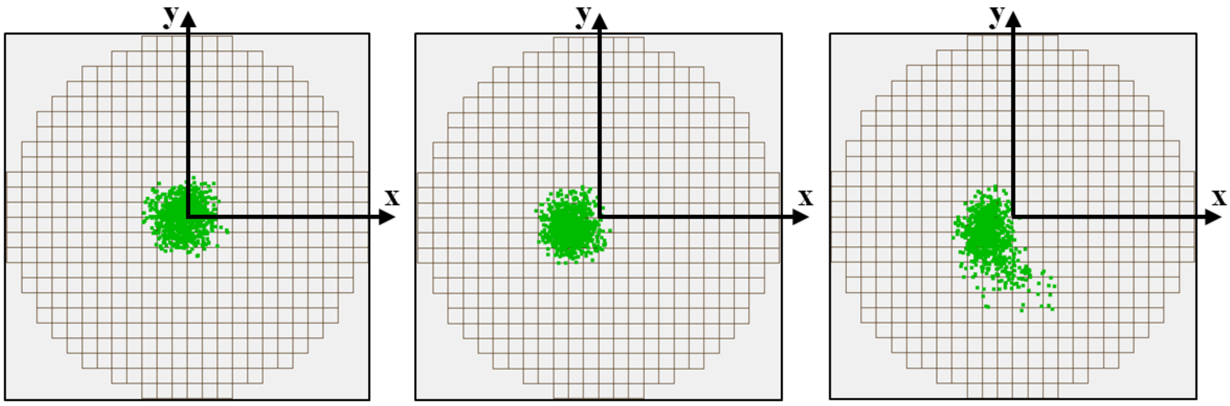


Fig.7. Distribution of positron beam on the target of the 90^0 bent-shaped model in case of solenoid deviation of 0 cm (left), 1 cm (middle) and 2 cm (right)

3. CONCLUSIONS

We have come up with the selection of the 50^0 bent-shaped model as a conceptual design for our slow positron beam system based on simulation test results and consideration of the design feasibility of the simulation models. The proposed model can be a good basis for detailed engineering design and construction of the system in the future. The study results have also demonstrated that Simion program is a very suitable tool for modeling and simulation of the trajectory of positron beam flying through electrostatic fields and magnetic fields of a slow positron beam system. Research of searching for other simulation programs to combine with Simion should be done to further optimize the conceptual design.

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THIẾT KẾ NGUYÊN TẮC HỆ THỐNG CHÙM POSITRON CHẬM BẰNG CHƯƠNG TRÌNH MÔ PHỎNG SIMION

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Tóm tắt: Hệ thống chùm positron chậm là một thiết bị quan trọng trong nghiên cứu vật lý và kỹ thuật positron, đặc biệt được ứng dụng trong nghiên cứu vật liệu. Báo cáo của chúng tôi trình bày các kết quả nghiên cứu và áp dụng chương trình mô phỏng quỹ đạo hạt mang điện Simion để xây dựng các mô hình thiết kế khả thi cho hệ thống. Một số tính toán mô phỏng thử nghiệm quỹ đạo chuyển động của chùm hạt positron đã được tiến hành nhằm mục đích so sánh giữa các mô hình. Từ đó, một mô hình thiết kế nguyên tắc đã được đề xuất để làm cơ sở cho việc xây dựng hệ thống chùm positron chậm thực tế trong tương lai ở Việt Nam.

Từ khoá: *Hệ thống chùm positron chậm, chương trình mô phỏng, Simion, thiết kế nguyên tắc*