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Some initial results of simulating a positron beam system by using SIMION

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Abstract: Slow Positron Beam (PB) is an important device in the study of positron physics and techniques, especially in material research. For the purpose of conceptual designing a PB system, we have simulated a PB system with the parameters of an existing system – SPONSOR, using SIMION software. The simulation results have been compared with the SPONSOR published results. The effect of magnetic field in controlling beam trajectory has been investigated in the pre-accelerated and accelerated stages. The simulation results of using steering coils to adjust the beam trajectory are also presented in this report.

Keywords: *SIMION, positron beam, simulation*

I. INTRODUCTION

Positron annihilation techniques play an important role in the study of micro-defect of materials, nano structures, porous materials, surface analysis, etc.[1]. However, the study of surface structure, layers or interface regions can not be performed with traditional isotopic 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). To solve this problem, positron beam (PB) stems have been developed. They are applied widely in materials science, physics of solid state, condensed matter and surface [2-3]. In general, most of the PBs has similar operating principle. A number of the high energy positrons emitted from the radioactive source are slowed down (moderated) to the eV range by the moderator and become slow positrons. The slow positrons are then separated from the high energy positrons, pre-accelerated to several tens of eV to create a mono-energetic positron beam, and are guided in a vacuum system to an accelerator. They are accelerated from several tens eV to several tens keV, and then are directed to the sample chamber and interact with the sample. The features that distinguish the PBs are the selection of moderator, method of slow positron beam extraction and acceleration. In order to make good and effective use of a PB, it needs to be designed and constructed properly, especially when the PB uses positron isotopic sources such as Na-22.

The use of a charged particles trajectory simulation program is an essential prerequisite to ensure the quality of the conceptual calculation and design for a slow positron beam system. Method of simulating

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trajectory of charged particles in electromagnetic fields has been applied for ages in design calculation of slow positron beam systems in the world. SIMION is a highly interactive simulation program used to model ion optics problems including simulating and calculating electrostatic fields, magnetic fields and the trajectories of charged particles flying through those fields [9-10]. SIMION has been used widely and effectively in many typical research projects on designing and building slow positron beams at 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 [1,10-13]. That was the reason why we chose SIMION to use as the main tool to model and simulate for the purpose of conceptual designing a PB system.

SIMION (Version 8.1) is a software package used primarily to calculate the electric fields and trajectory of charged particles in these fields when introducing the electrode configuration with voltage and initial conditions of the particles. In particular, SIMION provides functions of extensive support in the definition of geometry, user programming, data logging and visualization.

We are currently proposing a research project to design and build the first PB in Vietnam. If the project is approved and funded, the PB will be constructed and installed at the Center for Nuclear Techniques (CNT), Ho Chi Minh City. This PB, combined with positron annihilation spectroscopy currently available at CNT, will enhance the research and application of positron technology in Vietnam, especially in materials research in industry and environmental protection. In this paper, we present some primary simulation results for a PB system using SIMION software (Version 8.1) [9-10] and SPONSOR-PB published parameters [4, 11].

II. SIMULATIONS

The Slow Positron System of Rossendorf (SPONSOR), at Institute of Radiation Physics, Helmholtz-Centre Dresden-Rossendorf, Germany [11], is a very good working experimental setup example of a slow positron beam system with simple design principle. For many years, the PB has been operating well and effectively used for solid surface investigations. The operation principle of this system is illustrated in Figure 1. The schematic arrangement of magnetic guidance coils of it is given in Figure 2. A set of magnetic guidance coils, comprising nine solenoids and two pairs of Helmholtz coils, is arranged along the beam axis for achieving a nearly constant axial magnetic flux density of 100 Gauss. Additional windings of wire are applied on both ends of each solenoid (except for solenoid S6) to compensate the decrease of magnetic flux density between adjacent coils.

We have been performing some tests using a set of published data for this system. Our work has been modeling and simulating some components of SPONSOR system and calculating some parameters specific to the electrostatic and magnetic fields in the system as well as trajectories of a slow positron beam in the magnetic field. The components of the PB system, which have been simulated, included the solenoid and Helmholtz coils, the pre-accelerator and the accelerator stage. The data obtained from the simulation have been compared with the original data and the necessary corrections have been made. To improve the positrons arrival ratio at the target, the steering coils have also been simulated, and their design parameters have been determined.

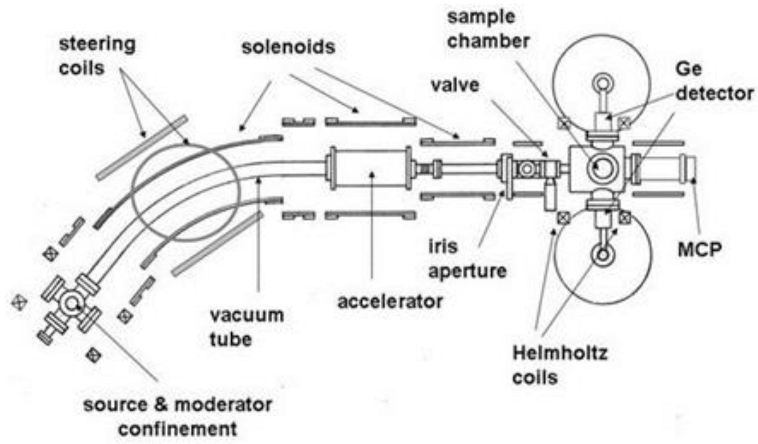


Fig. 1. Schematic outline of SPONSOR system

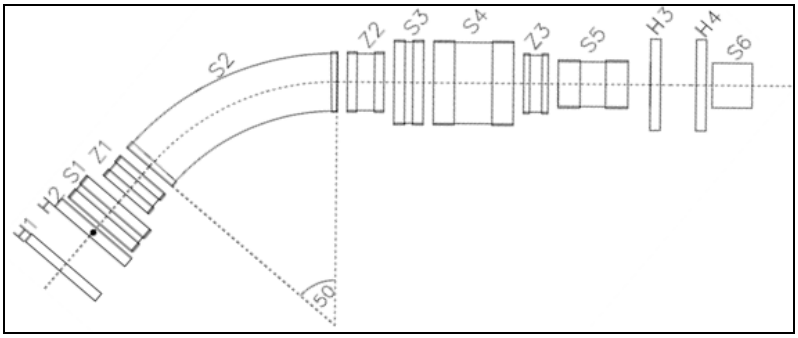


Fig.2. Schematic arrangement of magnetic guidance coils of SPONSOR system
(Here S and Z implies for solenoid coils, H- Helmholtz coils)

III. RESULTS AND DISCUSSION

A. Modeling the magnetic guidance coils

The schematic arrangement of magnetic guidance coils of SPONSOR system was modeled within SIMION. Some coils with experimental values of measuring the axial magnetic flux density have been chosen as representiative coils to model and simulate. These coils includes the first Helmholtz coil H1, the first solenoid S1 and the solenoid S4 enclosed the accelerator. The reference parameters are given in Table I.

Table I. Parameters of some representative coils used for modeling

Coils	Length (cm)	Inner radius (cm)	Current (A)	Number of windings per layer	Number of layers	Diameter of copper wire (mm)
H1	5	25	5	24	24	2
S1	14.5	20	5	69	4	2
S4	40	20	5	208	4	1.8

The calculation of axial magnetic flux density (Bz) along the axis (Oz) of these individual coils have been carried out with a 5A DC current source. The results for the H1, S1 and S4 coils are given in Table II. The results show that there are some differences between our simulated values and experimental values measured for the SPONSOR. However, in all the cases the differences are acceptable (smaller than 5%). The simulation results also show that in order to obtain the uniformity of the magnetic field along the path of the positron beam, the DC currents supplied to the coils must have been chosen appropriately. In the design of SPONSOR, current values of 3, 4, and 5A have been used, which have generated fairly uniform magnetic density. The results are shown in Figure 3. By adjusting parameters of the coils such as supplied currents, number of windings, a nearly constant flux density of 100 Gauss has been obtained over a length of 3.0 m along the path of the positron beam.

Table II. Axial magnetic flux density along the axis the coils
Bz (SPON)-Values of SPONSOR, Bz (SIMI)-Value calculated by SIMION

Distance (mm)	H1			S1			S4		
	Bz (SPON) (G)	Bz (SIMI) (G)	Difference (%)	Bz (SPON) (G)	Bz (SIMI) (G)	Difference (%)	Bz (SPON) (G)	Bz (SIMI) (G)	Difference (%)
0	68.6	71.5	*4.2*	40.0	40.2	*0.5*	91.4	91.6	*0.2*
50	61.7	63.7	*3.2*	37.0	37.4	*1.1*	89.1	89.4	*0.3*
100	49.6	51.8	*4.4*	30.0	30.7	*3.3*	81.1	82.9	*0.4*
150	37.9	39.8	*5.0*	22.0	22.8	*2.3*	71.4	72.1	*1.0*
200	30.1	29.7	*1.3*	16.0	16.2	*1.3*	56.6	58.2	*2.8*
250	21.8	22.0	*0.9*	11.0	11.3	*2.7*	43.9	43.9	*0*
300	17.1	16.4	*4.1*	8.0	7.8	*2.5*	32.6	31.7	*3.1*
350	11.8	12.3	*4.1*	5.5	5.5	*0*	22.9	22.5	*2.8*
400	9.3	9.4	*1.1*	4.0	4.1	*2.5*	16.3	16.1	*1.2*

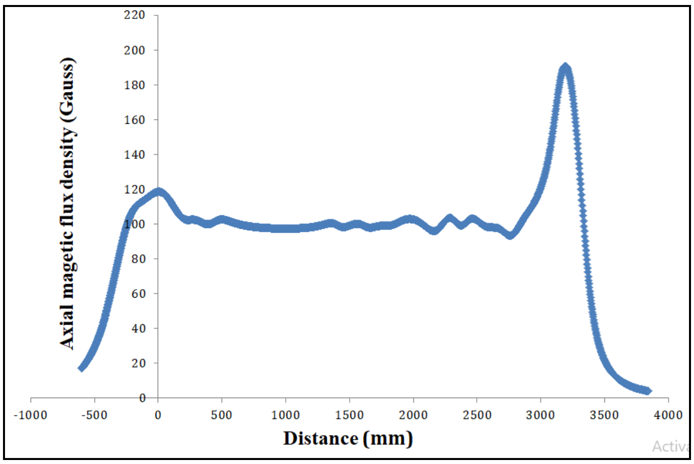


Fig. 3. Calculated magnetic flux density created by all of the coils. The currents of 3, 4, and 5A have been appropriately selected for each coil to give a fairly uniform magnetic density

B. Modeling the pre-accelerator and the accelerator stage

The pre-accelerator stage locates behind the thin Tungsten film moderator that helps to form and pre-accelerate the moderated positron beam by using spherical Wehnelt electrodes to create electrical field [12]. The positron trajectories in the pre-accelerator have been investigated. SIMION has been used to calculate the trajectories for 100 mono-energy positrons in a beam emitted from a circular uniform distribution source with a diameter of 2 mm, an initial kinetic energy of 3 eV flying through the modeled pre-accelerator. The positrons in the beam are emitted in the same direction parallel with the beam axis. The simulations have been done in two conditions, without and with magnetic field and the results are given in Figure 4. The kinetic energy of the beam could reach up to about 30 eV at the exit of pre-accelerator stage. The results in Figure 4(b) show the important effect of the uniform magnetic field in maintaining the diameter of the beam.

(a) **(b)**

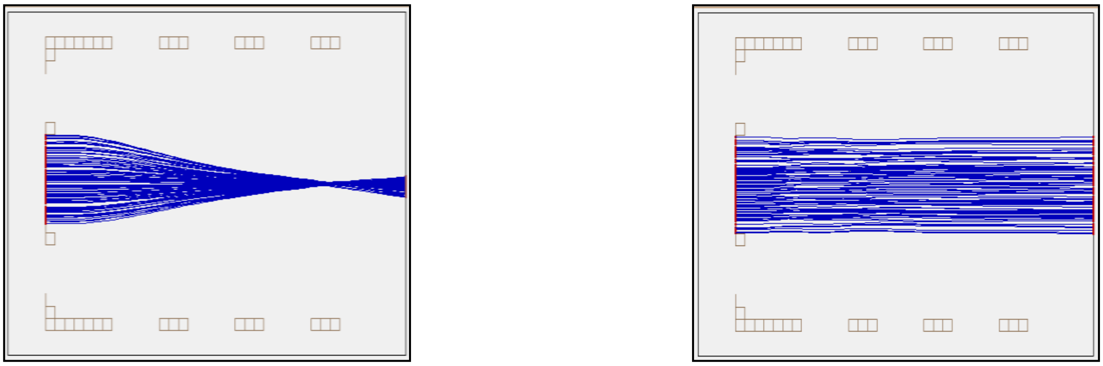
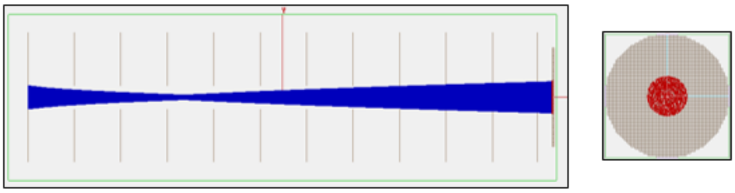


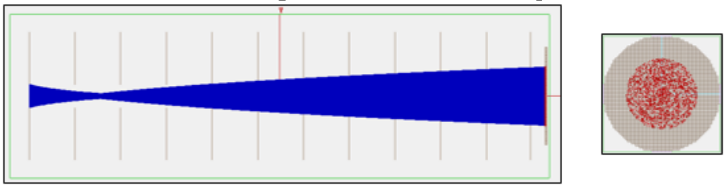
Fig. 4. Trajectories of the positrons (3 eV) flying through pre-accelerator without (a) and with a uniform magnetic field of 100 Gauss calculated by SIMION (b)

The accelerator stage consists of 12 electrode plates with 15 mm - diameter hole in the center. The plates are equidistantly spaced and the distance from one to another is 30mm. The power supply for the accelerator stage can be adjusted to give a high voltage output up to 50 kV. This means that the positron can be accelerated up to 50 keV. The trajectories for 2000 mono-energy positrons in a beam emitted from a 7 mm - diameter source in the same direction parallel with the beam axis with the initial kinetic energy of 3eV flying from the entrance to the exit of the accelerator without magnetic field are shown in Figure 5 a, b, and c for cases of high voltage of 1 kV, 20 kV and 50 kV, respectively.

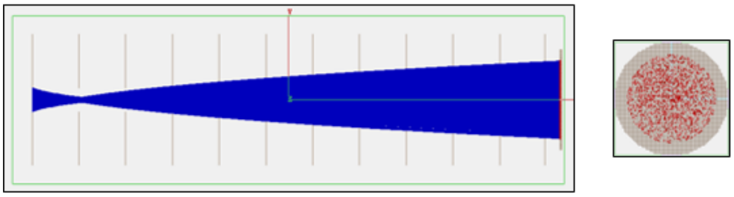
It is clear that the high voltage of the acceleration strongly influences the movement of the positrons in the absence of magnetic field. The electrostatic field created from the electrode plates focuses the positron beam flying through the accelerator. When the high voltage increases, the focusing point is nearer the entrance of the accelerator. That makes the size of the beam spot increases as the high voltage increases. In case a uniform magnetic field was superimposed on the electrostatic field in the acceleration region, the cross section of the beams would vary much less in comparison with the above case (with no magnetic field). This effect is demonstrated in Figure 6. When a uniform 100 Gauss magnetic field was applied on to the accelerator stage with 50 kV high voltage, the radius of the beam spot decreased from 22.6 mm to 7.1 mm. The value of 100 Gauss for the uniform magnetic field could be a good choice for the design because it would help maintain the beam diameter small enough to safely pass through the 15mm – diameter holes at the center of the accelerator electrode plates.



a) Trajectory of a 3eV positron beam inside the accelerator with a high voltage of 1kV and the distribution of the beam at the target, radius of the beam spot-9.3mm



b) Trajectory of a 3eV positron beam inside the accelerator with a high voltage of 20kV and the distribution of the beam at the target, radius of the beam spot-17.5mm



c) Trajectory of a 3eV positron beam inside the accelerator with a high voltage of 50kV and the distribution of the beam at the target, radius of the beam spot-22.6mm

Fig. 5. Trajectory of a positron beam (3eV) inside the accelerator with different high voltages and no magnetic field

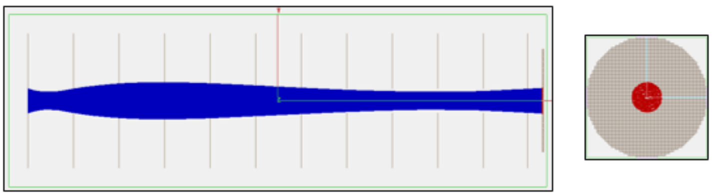
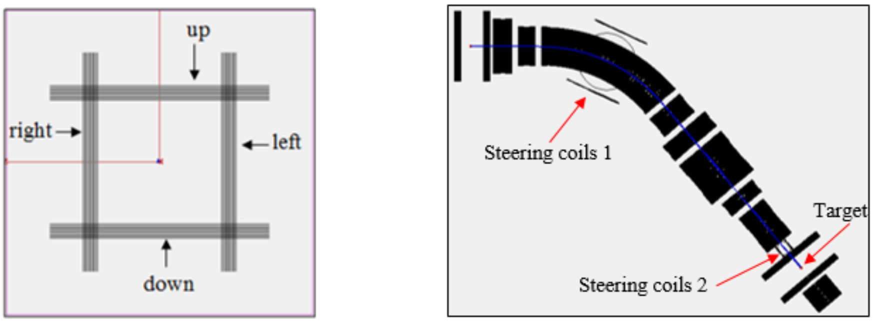


Fig. 6. Trajectory of a positron beam (3eV) inside the accelerator with a high voltage of 50kV and a uniform magnetic field of 100 Gauss and the distribution of the beam at the target, radius of the beam spot-7.1 mm

C. Modeling the steering coils

If the system consists only of solenoid coils, pre-accelerator and accelerator stage, a large portion of slow positron beam can not reach the desired spot on the target at the sample chamber because they will interact with the wall material of the guiding tube. The reason is that there are small deviations of the beam axis from the center line caused by the non-uniform magnetic field in the tube segment that is bent to filter the slow positrons. The influence of centrifugal force and the oscillation of the beam after passing the accelerator also contribute to the deviation of the beam [4,13]. Calculations with SIMION have showed that only about 25% of the slow positrons would pass through the accelerator to reach the target, while the rest have been lost due to collisions with the accelerator plates. To adjust the beam axis, two pairs of steering coils were added to the PB system for simulations. Steering coils 1 located at the bent section and steering coils 2 were in front of the sample target. They were parallel to the beam line.



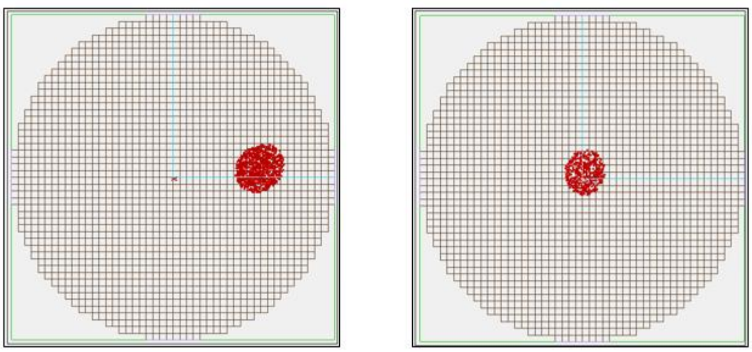
(a) (b)

Fig. 7. Arrangement of two pairs of steering coils **(a)** and positions of steering coils modeled by SIMION **(b)**

Currents for each of the steering coils could be tuned appropriately and carefully to create a combination of magnetic field that moved the beam correctly in horizontal and vertical directions. The appropriate parameters of the coils are given in Table III. The distribution of mono-energy positrons at the sample target without and with the steering coils is shown in Figure 8. From the results it can be concluded that the use of steering coils is necessary in adjusting the trajectory of the positron beam so that it can reach the desired target.

Table III. Parameters of modeled steering coils

Parameters		Length (mm)	Inner radius (mm)	Current (A)	Number of layers	Total number of windings	Diameter of copper wire (mm)	Distance from the beam line to center of the coil to (mm)
Steering coils 1	up	10	220	0	1	10	2	285
	down	10	220	6.25	1	10	2	285
	left	10	220	9	1	10	2	285
	right	10	220	0	1	10	2	285
Steering coils 2	up	10	50	0	1	10	2	45
	down	10	50	2.5	1	10	2	45
	left	10	50	8	1	10	2	45
	right	10	50	0	1	10	2	45



(a) (b)

Fig. 8. Distributions of positrons at the sample target without steering coils **(a)** and with modeled steering coils **(b)**

IV. CONCLUSIONS

The simulation results of the preliminary test for SPONSOR system have demonstrated that SIMION can simulate accurately and quickly the behavior of a positron beam in electromagnetic and electrostatic fields. Simulation results show the importance of solenoid, Helmholtz, steering coils as well as magnetic fields in the control of the positron beam from the source chamber to the target. In order to successfully design and build a PB system, much work remains to be done. The tasks to be performed will include optimizing the curvature of the beam line to increase radiation safety, selection of the parameters for the solenoid coils that surround the bent segment of beam tube to generate uniform magnetic field, etc. If the partially finished beam device in CNT given by Hungarian is to be used, the accelerator stage with only five voltage stages (six plates) must also be modeled and simulated.

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