SIMION simulation of a slow pulsed positron beam*

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Abstract: A new slow pulsed positron beam, including a positron source, a moderator, a chopper, a pre-buncher, a main-buncher and a sample chamber, etc, has been installed and tested. It is necessary to simulate the acceleration, transportation and space focusing of positrons to meet the needs of beam debugging and further positron annihilation experiments. The result from SIMION simulations shows that the radius of the focused positron beam is less than 5 mm, which is further confirmed in our practical debugging process.

Key words: annihilation, slow pulsed positron beam, simulation

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1 Introduction

Positron annihilation technology (PAT) is a very sensitive and non-destructive detecting tool in studying the micro-defects of materials [1–5]. Due to the broad energy distribution of the source-emitted positrons and the broadened penetration depth in the samples, the traditional positron life spectrum, Doppler broadening spectra and angular correlation spectrometer cannot be used to probe the defects in surface or interface regions. Thus the slow positron beam has been designed and the results indicate it is effective in detecting the surface microstructure of the samples [6, 7]. Since there are many advantages of slow positron beams, such as the fact that it is sensitive and non-destructive in detecting atomic scale defects in surfaces or interfaces, the technology has been widely used in solid state physics, surface physics, condensed matter physics and material science [2–4]. There have been several slow positron beams in the world [8–12]. Our laboratory built the first slow positron beam using a ^{22}Na source in China as early as 1990 [6]. If the slow positron beam were pulsed further, the depth-dependent positron annihilation lifetime could be measured, which is impossible to realize in non-pulsed positron beams. In addition, the Doppler broadening spectrum and age-momentum correlation spectrum could be detected simultaneously to characterize the material's surface microstructure more effectively. Thus a new slow pulsed positron beam has been designed and tested since 2007 in our laboratory.

The space-focusing of the beam is crucial for beam debugging and positron annihilation experiments. In this work, an ion optics simulation software called SIMION [13] is introduced briefly. Then the space-focusing of the slow pulsed positron beam is simulated by SIMION and some essential parameters are obtained. In addition, the result of debugging with an electron gun on the beam is coincident with our SIMION simulation.

2 The physical model and the SIMION simulation software

2.1 Physical model

A schematic overview of our slow pulsed positron beam is shown in Fig. 1. The common slow pulsed positron beam often includes a positron source, a W-moderator, lead shielding, a chopper, a pre-buncher,

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a main buncher [8–12, 14], an accelerator, a sample chamber, etc. The high-energy positrons emitted from the source are moderated as slow positrons by the tungsten mesh moderator, and then the slow positrons are extracted by an extracting electrode with an energy of about 24 eV. The slow positrons are transported through the guidance of a 5×10^{-3} T magnetic field, which is achieved by 14 groups of coaxial solenoid coils positioned on the axis of the beam. On its way, a chopper, including three layers, is applied with an approximate rectangular wave signal (50 MHz frequency) to make the continuous positron beam turn into a pulsed positron beam. The chopped positron beam (with a time window of 5 ns) reaches the pre-buncher (50 MHz frequency) and main buncher (200 MHz frequency), which are applied with a sine signal wave and can compress the slow pulsed positron beam to become much narrower (120–150 ps in FWHM). Finally, the slow pulsed positron beam is accelerated by the accelerating electrodes and hits the sample target. Positron annihilation experiments such as the positron annihilation lifetime spectrum, the Doppler broadening spectrum, the coincidence Doppler broadening spectrum and the age-momentum correlation spectrum can be measured on this apparatus at the same time.

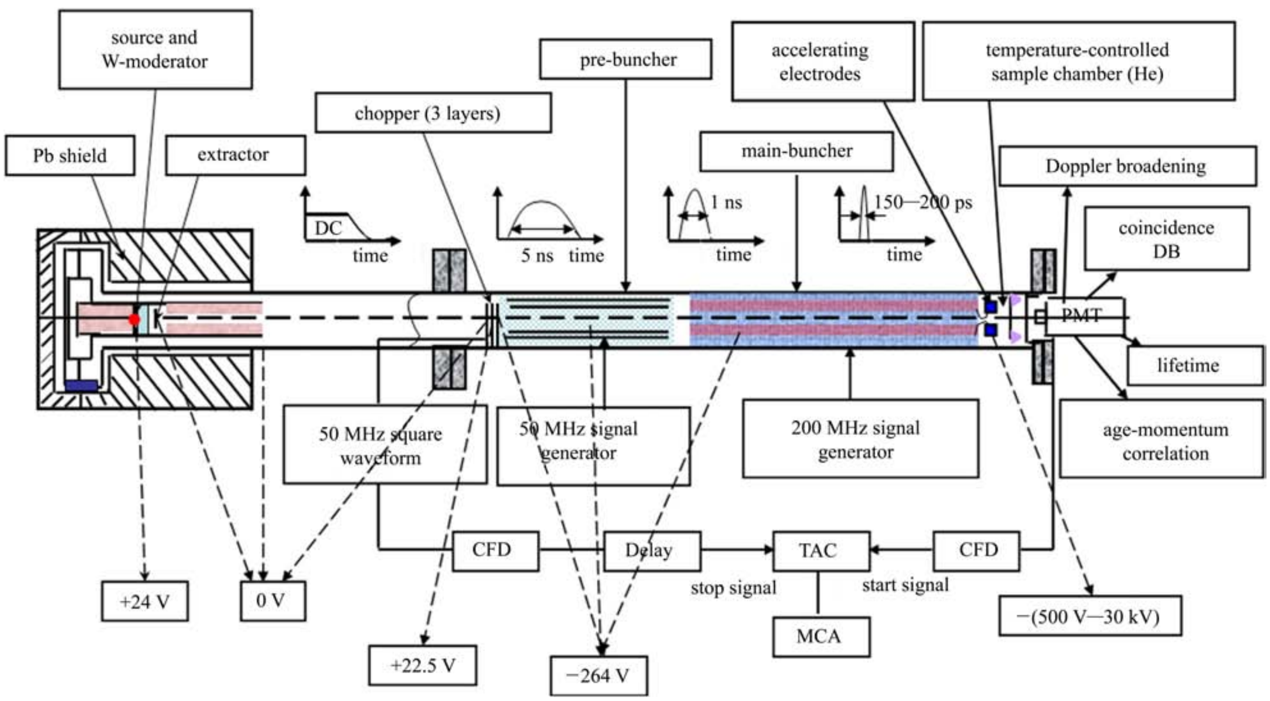

Fig. 1. Schematic diagram of a slow pulsed positron beam.

2.2 The SIMION simulation software

SIMION is well known as a kind of ion optics simulation software that has been widely used since it was first introduced in 1986 [13]. It can calculate electric fields and give the trajectories of charged particles in electric or magnetic fields to analyze ion characteristics in 2D or 3D coordinates when the voltage of the electrodes and initial conditions (including optional RF, magnetic field, collision effects, etc.) are given. In addition, it can simulate time of flight, mass spectrometry, quadrupole, ion source, optical detector and other more complex physical models [13, 15].

The SIMION simulation software is robust, easy and flexible to use due to its interactive graphic user interface (GUI), user programming and ion trajectory visualizations, which significantly enhance the power and versatility of SIMION. There are many parent-child related graphical objects based on their functions which make the communication between the user and objects more convenient, powerful and efficient.

User programming allows the user to write a program associated with the designated potential arrays in a reverse polish notation (RPN) language. SIMION can compile and incorporate these programs into the ion flying process automatically.

SIMION's maximum simulation universe is 8 km^3 in cubic volume and its actual simulation bench-ion optics workbench has a volume that resides within that universe. All the features of ion can be obtained within the workbench. SIMION's visualization software employs floating point vector graphics to permit a wide range of workbench volumes viewed in full screen, from a cubic micron to a cubic kilometer, which makes the complex ion motions visual and intuitive.

Both the electric and magnetic fields are used in our slow pulsed positron beam spectrometer. In addition, a positron is a kind of charged particle, so SIMION could be used to simulate the process of positron transportation, acceleration and space focusing in the apparatus.

3 The simulation process

Generally speaking, the fundamental step to simulate a positron beam is to determine the corresponding parameters, such as the electric fields, the magnetic fields and the initial conditions of the positrons. Then the trajectories can be obtained.

3.1 Creating an electrostatic potential array

SIMION uses the potential array approach to calculate the electronic fields, up to 50 million points can be refined as a potential array. Each potential array that represents every part of the instrument is placed in the ion optics workbench, the extension file names of which are usually .PA, .PA# or .PA0.

Creating a new potential array named test1.PA# and inserting the electrode geometry according to the schematic diagram of the slow pulsed positron beam is shown in Fig. 1. The voltage of each electrode is given as follows. The voltage applied to the moderator is 24 V. The voltage applied to the extractor, Pb shield and the transportation vacuum tube is 0 V. The voltages applied to the first, second and third layers of the chopper are 0, 22.5 and −264 V, respectively. Both the pre-buncher and main buncher are applied a voltage of −264 V. The voltage applied to the Faraday cup and sample chamber varies from −500 to −30 kV.

3.2 Creating a magnetic potential array

SIMION can solve a restricted instance involving scalar magnetic potential, Biot–Savart wire calculations or other magnetic fields by importing files from an external program [13]. In this simulation, the magnetic field is achieved by 14 groups of coaxial solenoid coils accurately positioned on the z-axis. According to the location, radius, length, density of coaxial solenoid coil and the magnetic field spiral formula of finite length solenoids [see Eq. (1)], a magnetic field document named Mag. PRG is compiled.

$$B=\frac{\mu_0 N}{2}\left\{\frac{l_2-z}{\sqrt{R^2+(z-l_2)^2}}-\frac{l_1-z}{\sqrt{R^2+(z-l_1)^2}}\right\}, \tag{1}$$

in which, R is the radius of the coil, l_2 and l_1 are the right and left coordinates of one coil in the beam, respectively, z is the coordinate of the moving positrons in the beam, N=$n\times I$, n is the number of turns in the coil per meter (fixed) and I is the electric current of the coil.

3.3 Flying positrons

In this research, three groups of positrons were chosen, the coordinates x, y and z of each group are set as follows: (0, 5, 0 mm), (0, 0, 0 mm) and (0, −5, 0 mm), the emission angles of the positrons in each group are 7°, 0° and −7°, and the file is named as Positron. Fly after these parameters of positrons are defined.

Once the electric potential array, magnetic potential array and the positron's parameters are defined, the positrons can be flown separately or simultaneously in groups through the ion optics workbench.

4 Results and discussion

During the simulation, the N parameter is adjusted, which causes a change in the magnetic field intensity B and the trajectories of the positrons. In addition, the positron drifting, transportation and focusing profile in the ion optics workbench are calculated and obtained through the SIMION visualization software, as shown in Fig. 2.

As shown in Fig. 2 (a) and (b), positrons are first emitted from the ^{22}Na and extracted to the transportation vacuum tube. Then they get across the chopper, pre-buncher and main-buncher to turn into pulsed positrons through the guidance of a 5×10^{-3} T magnetic field, and finally the pulsed positrons are accelerated by the accelerating electrodes with the energy adjusted from 500 eV to 30 keV and focused on the target.

According to the positron simulation experience with SIMION, we know that the more uniform the magnetic field is, the better the focusing result, so both the homogeneity of the magnetic field and the focusing radius must be taken into account in the regulation of the N value. In addition, the current I value of the coil cannot be too high, otherwise it will increase the energy consumption and reduce the service life of the high voltage power.

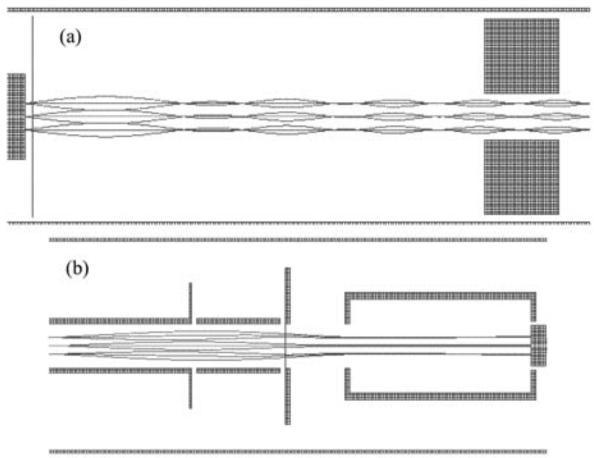

Fig. 2. The processes of positron transportation (a) and focusing on the target (b).

With the above simulation experience, the space focusing of the slow pulsed positron beam with an energy range of 0.5 to 30 keV is simulated and the optimal parameters of the coils are listed in Table 1. The calculated magnetic field intensity B for our beam is about 5×10^{-3} T. 6375 or 5090 is the N parameter of the first coil when the positrons are accelerated to 0.5–5 keV or 5–30 keV, respectively. Since the length, density and radius of the coils are fixed, with N parameters, the electric current (I) of each coil can be calculated easily and the positron beam can be tuned with these parameters in next step.

Table 1. The parameters of the coaxial solenoid coils.

coil number	radius/mm	length/mm	$N=$ (n$\times I$)
1	125	132	6375 or 5090
2	65	43	8628
3	65	43	8628
4	65	43	9361
5	65	43	8628
6	65	43	9361
7	65	43	8628
8	65	43	8140
9	65	43	8140
10	120	43	5291
11	120	43	5291
12	65	43	8628
13	120	43	6186
14	105	43	6186

The variation in positron focusing radius with accelerated energies is obtained in the ion optics workbench and shown in Fig. 3. It is found that the spatial focusing radius shows as a function of the accelerated voltage. The focusing radius of the positrons in the beam is controlled at less than 5 mm, which meets the need of our positron experiments. With one group of coil parameters shown in Table 1, the focusing radius decreases quickly with the increase in accelerated voltage. However, when the accelerated voltage is above 25 kV, the radius shows small differences, which is in accordance with our testing results introduced below.

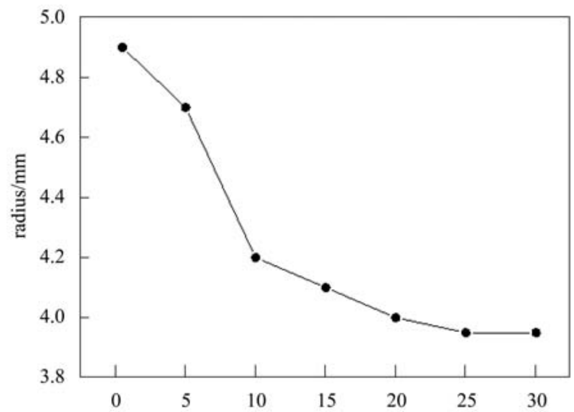

Fig. 3. The variation in focusing radius with accelerated energies.

Fig. 4. The practical profile of the electron beam spot in our pulsed positron beam device.

An electron gun replacing the ^{22}Na source is used to debug the slow pulsed positron beam. A position-sensitive detector composed of a micro channel plate (MCP) and a fluorescent screen is placed in the sample chamber, and thus the electron beam spots could be observed through the window on the flange. By adjusting the current value of each coil according to the parameters listed in Table 1, a clear, bright and small electron beam spot located roughly in the center of the fluorescent screen is obtained. The practical electron beam achieved in our device with the measured profile is shown in Fig. 4, from which it can be concluded that the SIMION simulation result for the beam is inspiring and that the practical space-focusing debugging of the beam is coincident with the simulation result.

5 Summary

SIMION is used to simulate the space focusing of a slow pulsed positron beam, and the desired simulation result meeting the needs of experiments is obtained. Basic installation and space-focusing testing with the electron gun on the spectrometer were successfully completed, and the result of space-focusing in the beam after testing and debugging is coincident with our SIMION simulation result. The practical profile of the electron beam spot observed by an MCP in our device is small and bright enough. Testing and debugging of the time-focusing are now being performed on our beam device, and the ^{22}Na source will then be used to adjust the beam with the help of the simulated coil's parameters.

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