GEANT4 SIMULATION OF POSITRON LIFETIME IN MATERIALS

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Abstract: GEANT4 (GEometry ANd Tracking) is an object-oriented Monte Carlo simulation toolkit to simulate the passage of particles through matter. This research was carried out to model a system for measuring positron lifetime in materials by GEANT4 whereby the nature of positron annihilation in material was understood clearly. The specific details of ^{22}Na source which emitted positrons with its energy in a 0-545 keV range was reproduced by GEANT4. Based on the positron annihilation in the sample, the penetration and the lifetime of positron were investigated. Besides, the experimental measurements of the lifetime positron in some metals, such as Cu, Al, Fe and Ni, were also conducted at Center for Nuclear Techniques. After all, the GEANT4 simulation results have been compared to that of experiments. The results show that the positron energy distribution of ^{22}Na source in GEANT4 is compatible with the published articles. The positron penetration in the samples, in simulation and experiment, have also the same results. The spectrum form of the positron lifetime in Cu, Al, Fe and Ni simulated in GEANT4 have a remarkable agreement with those of measured results. The system measuring directly positron lifetime, which has been simulated successfully, shows that using GEANT4 to evaluate the differences between experiment and theory of positron annihilation is essential for the material science field in particular and the physics in general.

Key words: positron annihilation, GEANT4.

1. INTRODUCTION

Positron annihilation lifetime spectroscopy (PALS) is a non-destructive spectroscopy technique that allows us to study a wide range of phenomena and material properties on an atomic scale. PALS measures the elapsed time between the implantation of the positron into the material and the emission of annihilation radiation. The lifetime of the positron can thus be used to determine the pore size of the sample. Typical examples are smallest atomic defects in crystals, metals, semiconductors and polymers or chemical structures in fluids and biological systems.

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. It is based on 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 [1].

While there are a lot of the study on PALS over the world with GEANT4, simulating a positron lifetime system in materials have not been carried out in Viet Nam yet. Throughout the work of simulating a PALS, we could have a strong understanding of the nature of the positron annihilation in materials. Also, we could figure out some potential factors which affects to the results in experiments.

2. METHOD

In this paper, GEANT4 is used to simulate some sources emiting positron and define density of materials. After positrons have been annihilated in material, the information of its lifetime and implantation would been recorded immediately by GEANT4. ROOT tool is used to analyse the retained results from GEANT4.

Firstly, based on the real source in the experiments, the structure of sources, such as ^{22}Na, ^{26}Al, ^{44}Sc, ^{56}Co, ^{58}Co, have been built in GEANT4. The positron energy spectrum have been investigated and compared to the data of Eckerman et al [2]. The structure of sealed radiation source emitting positron is shown in Figure 1.

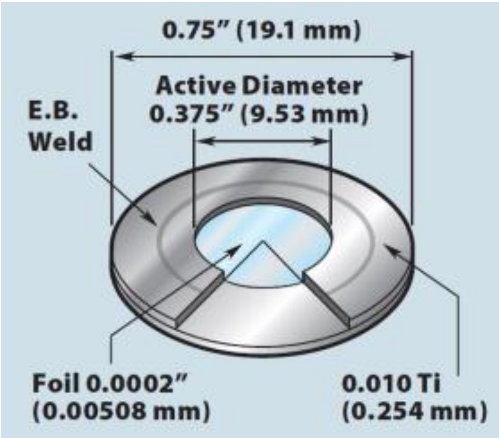

Figure 1: The structure of sealed ^{22}Na radiation source [3]

Secondly, a system consisting of a ^{22}Na source and a cylindrical solid materials with a radius of 5 mm and a thick of 2 mm was created in GEANT4 (described in Figure 2). The purpose of this model was to collect the positron implantation profile in different materials metioned in Table 1.

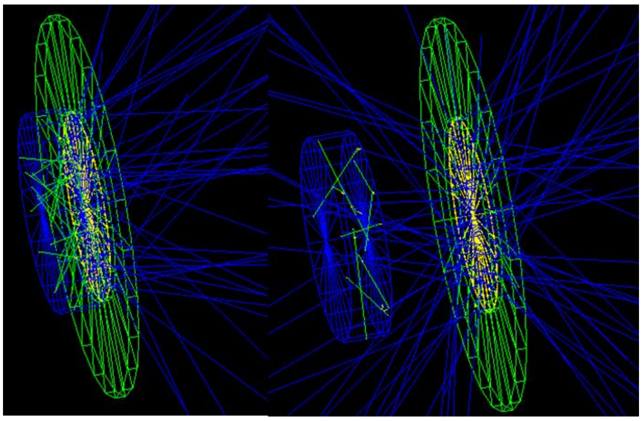

Figure 2: Radiation source and sample in GEANT4

Finally, we have contructed the model with a ^{22}Na source and two cylindrical solid metals in order to obtain positron lifetime spectrum. We also have conducted the experiment of measuring positron lifetime in Cu by the PALS in Center for Nuclear Techniques. The data from the simulation and the experiment have been compared to each other.

3. RESULTS AND DISSCUSION

To research the energy distribution of positron after being emitted from the different radiation sources, every source has been simulated to emmit 1000000 positrons. In this paper, ^{27}Al, ^{44}Sc, ^{22}Na are displayed in below Figure 3, Figure 4, Figure 5, in respectively. In each the picture, the left diagram is the result in GEANT4, the other is in the article of Eckerman et al.[2].

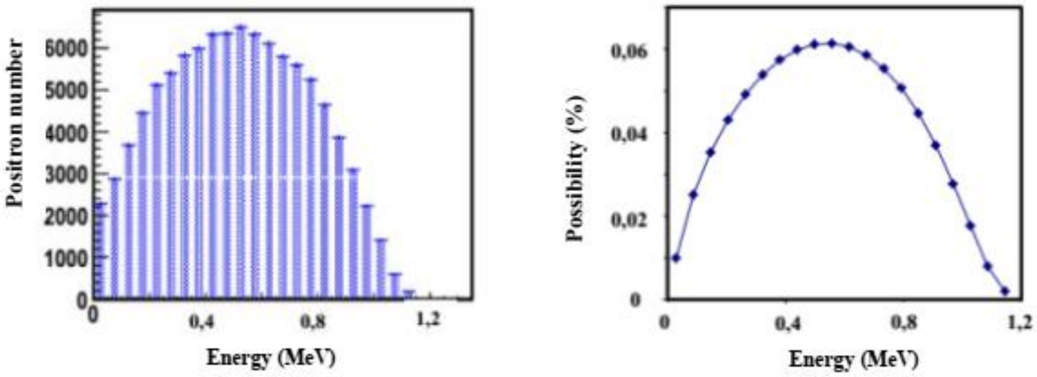

Figure 3: Energy spectrum of the positrons emitted by ^{26}Al source

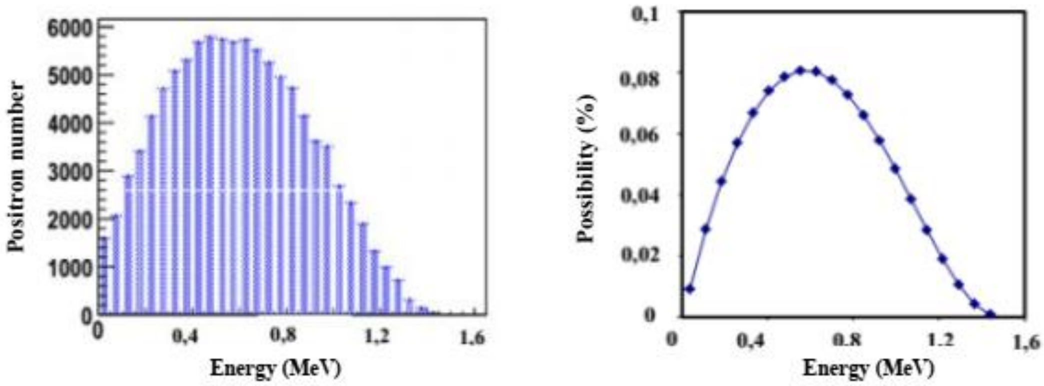

Figure 4: Energy spectrum of the positrons emitted by ^{44}Sc source

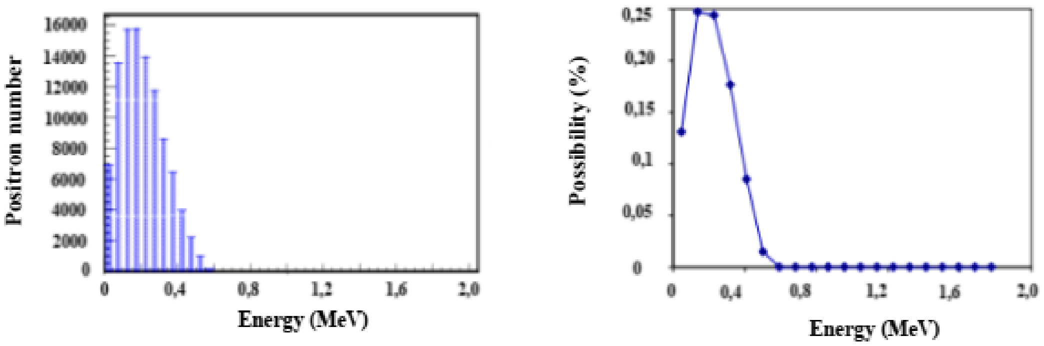

Figure 5: Energy spectrum of the positrons emitted by ^{22}Na source

The values of the mean positron penetration depth for different materials of different densities in GEANT4 have been recorded and shown in Table 1 below.

Table 1: The mean positron penetration depth for various materials in GEANT4

Material	Density (*g/cm*^{3})	Mean positron penetration depth (*mm*)	Annihilated positron number (over total 1 million of positron)
Paraffin	0,80	267,7 $\pm$ 2,6	27756
Polyethylene	0,92	236,4 $\pm$ 2,2	28981
Plexiglass	1,15	192,5 $\pm$ 1,6	32038

Kapton	1,42	169,1 ± 1,4	33260
Mg	1,74	134,6 ± 1,0	36525
S	2,07	105,2 ± 0,8	39777
Teflon	2,10	117,4 ± 0,8	38655
Graphite	2,26	103,3 ± 0,7	41347
Si	2,33	94,9 ± 0,7	41689
Glass	2,38	92,9 ± 0,6	42216
Al	2,68	86,8 ± 0,6	43680

To have a profound insight into the nature of positron annihilation in material, we have modeled two cases: in the first case, system consisting of one source and one metal sample, in the second case, one source is placed between two identical metal sample. While the value of lifetime positron is shown in Table 2, the spectrums of positron lifetime in GEANT4 in Cu sample are represented in Figure 6 and Ficture 7.

Table 2: The mean positron lifetime in GEANT4 with two different case

Material	**Case 1**		**Case 2**			
	Average positron lifetime (ps)	Event number	Average positron lifetime in sample 1 (ps)	Event number in sample 1	Average positron lifetime in sample 2 (ps)	Event number in sample 2
Al	6,230	45731	7,917	57763	7,837	57610
Cu	5,059	82009	7,187	112506	7,221	112332
Fe	5,120	77273	7,193	104944	7,172	104730
Ni	5,001	83989	7,153	115157	7,131	114942

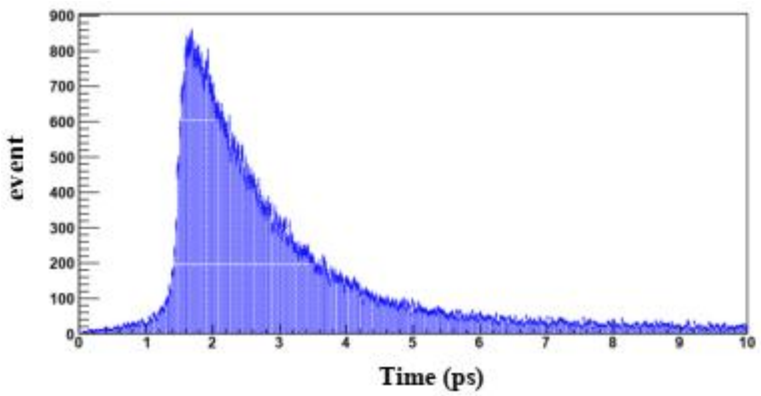

Figure 6: Positron lifetime spectrum in Cu sample in case 1

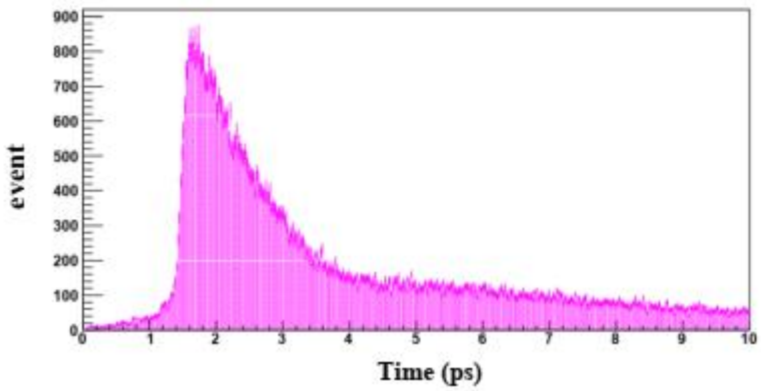

Figure 7: Positron lifetime spectrum in Cu sample in case 2

Besides the study with GEANT4, we also conducted an experiment of measuring the positron lifetime in Cu (pure copper) by PALS in Center for Nuclear Techniques in Ho Chi Minh city. The positron lifetime spectrum in this experiment is shown in Figure 8.

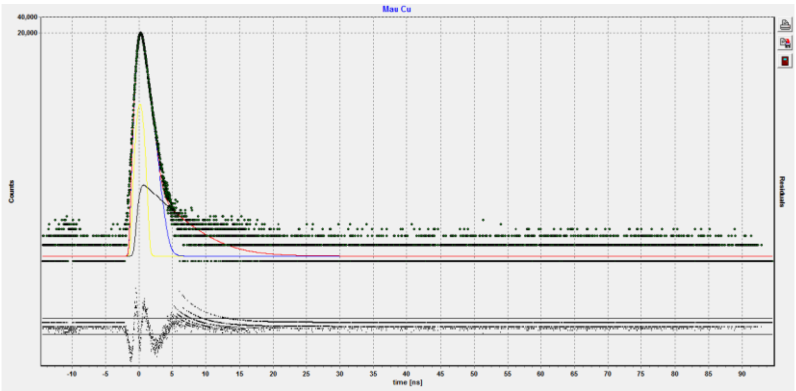

Figure 8: The experimental positron lifetime in Cu

The curve of positron energy distribution emitted from some radiation sources mentioned above (Fig 3, Fig 4, Fig 5) has a same form of one in the work of Eckerman et al . [2]. This is one of the most important results, thereby carrying out the next set up.

From the Table 1, the results show the relationship between the mean positron penetration and the material density in the Figure 9. It is well visible that the positron implantation range depends not only on the density of material but also the atomic number of material. This result has a good agreement with the experimental data of Dryzek et al. [4].

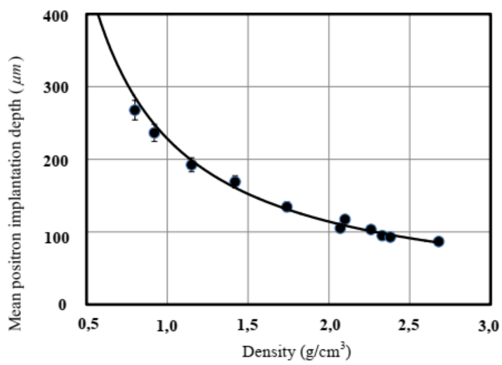

Figure 9: The dependence of the mean penetration depth as a function of the density of the measured materials taken from the Table 1

According to Mahmoud Hassan [5], positron annihilation lifetime spectrum in material is presented in Figure 10, it is evident that it reveals two decay constants: one corresponding to the lifetime in the bulk material and the other to the lifetime in defects. The relative amplitude of the two signals gives the density of the defects in the material, while the lifetime in the defects gives the defect size. We can see that the right part of the spectrum in Figure 7 is higher than that of the spectrum in Figure 6. It means that the annihilation lifetime of the positron in case 2 is longer than that of in case 1. One of the reasons causing that is due to the effect of compton scattering when two sample between a ^{22}Na source were modeled. Compared to Figure 10, it is a good fit if we only consider the form of these spectrum. While the time scale of the spectrum in GEANT4 is pico second, that of theory and experiment is nano second.

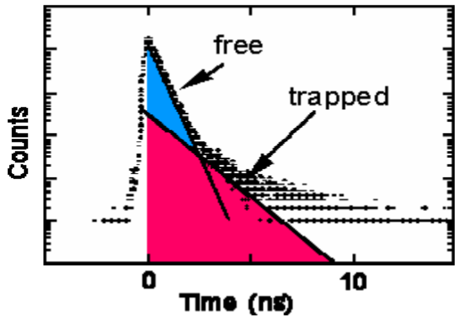

Figure 10: The number of positron decays as a function of time after entry into a material [5]

In futher study, to tackle this problem, we are going to build a other system including a ^{22}Na radiation source, two sample and two detector. Instead of receiving the lifetime of positron which being extracted from the data of proper time in GEANT4, we will base on the traced gamma (511 keV and 1274 keV) in order to calculate the positron lifetime. The obtained results will be considered carefully and compared to these results.

4. CONCLUSION

We have modeled a simple system recording the positron implantation profile and the lifetime of positron. Even though there are some problems needing to solve thoroughly, this research will open new using GEANT4 software in material investigation in Viet Nam.

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