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Calculation of Source Contribution using Particle Tracking Methods in Positron Annihilation Lifetime Spectroscopy

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1. Introduction

Positron annihilation lifetime spectroscopy (PALS) is a non-destructive technique for studying open-volume defects in materials such as pure metals, alloys, semiconductors, and polymers [1]. In PALS, a liquid form of the unsealed radioisotope (^{22}Na) is often selected as a positron emitter due to its limited penetration range in the matter. This liquid-based positron-emitting radioisotope needs to be encapsulated by a few-micrometer-thick foil to prevent contamination. Some of positrons annihilate in the source-supporting foil before reaching the samples. The source contribution, which involves positron annihilation within the source-supporting foil, is an inevitable aspect of PALS and requires correction for accurate analysis. This comprehension influences the precision of the analysis for positron lifetimes (τ) and relative intensities (I). In PALS, this source contribution ratio has been employed to rectify τ- and I-values for the samples.

Several researchers have studied this source contribution in PALS. The most widely used source contribution model was developed by Bertolaccini and Zappa; they only tested on three specific materials [2]. In addition, previous source contribution models were limited to the specific foil, such as the 7-µm thick Kapton foil. The Monte Carlo N-Particle (MCNP) simulation and its PTRAC feature are crucial in these assessments. The selective retrieval of particle trajectory data by PTRAC calls for further data processing. The aim of our study is to determine the source contribution of the 7.6-µm Kapton foil for various samples using MCNP PTRAC.

2. Materials and Methods

The positron source was shaped like a circle with a 3.5-mm radius. It was made to imitate the broad energy distribution from the ^{22}Na radionuclide. The ^{22}Na source was designed to emit positrons isotropically with an energy of 0.544 MeV at an 89.6% emission probability and gamma rays with an energy of 1.274 MeV at a 10.2% emission probability. The polyimide foil (Kapton foil) with H: 2.63%, C: 69.1%, N: 73.3%, and O: 29.2% supported the ^{22}Na source. The support foil had areas of 8×8 mm^2 and was 7.6-µm thick. In the geometry of that simulation, the ^{22}Na source was positioned at the center of the two support foils. The type of samples was Al, Ni, Zn, Zr, Sn, and W. They were designed with dimensions of 10×10 mm^2 and a thickness of 1 mm. The sample was placed on both sides of the centrally located support foils. Fig. 1. shows the geometry of the MCNP simulations. The PTRAC function was utilized in its bank (BNK) and termination (TER) modes to track and log all positron annihilation events.

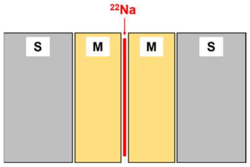

Fig. 1. Illustration of the modeled geometry on the Monte Carlo simulations. S: sample, M: 7.6-µm Kapton foil.

An empirical formula was introduced by Bertolaccini and Zappa as an illustrative example,

$$I = 0.324 \times Z^{0.93} t_m^{\frac{3.45}{Z^{0.41}}}$$

where the mass thickness t_m is in mg/cm^2, and the symbol Z is the atomic number of the sample. Once the MCNP simulation was completed, the generated PTRAC output files provided detailed records of individual particle histories. These files encapsulated every positron annihilation event throughout the simulation. This data set was processed using Python, as shown in Fig. 2, which shows the data processing workflow. The primary objective of the PTRAC results is to evaluate the source contribution by calculating the positrons that annihilated within the support foil out of the total annihilated positrons.

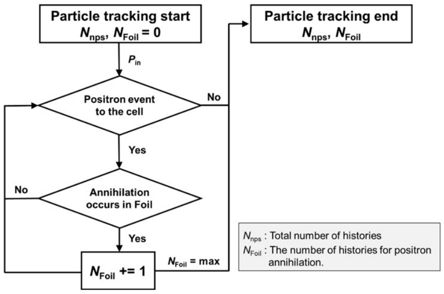

Fig. 2. Schematic diagram of the data processing of PTRAC output suing Python.

3. Results and Discussion

Fig. 3 presents a comparative analysis of the source contribution for 7.6-um Kapton foil compared with that from Bertolaccini and Zappa. The PTRAC result of the source contribution was larger by 0.38 for Al, 0.59 for Ni, 0.62 for Zn, 0.74 for Zr, 0.84 for Sn, and 1.07 for W times, respectively. The difference identified can be explained as follows: (1) a likely discrepancy arises because Bertolaccini and Zappa tested only three representative samples with $3 \leq Z \leq 6$. (2) the difference in the results of Bertolaccini and Zappa can be attributed to not considering the change in the backscatter coefficient of the positrons after they penetrated through the support foil.

The approach using PTRAC allows for considering the effects in the backscattering of positrons. Disregarding backscattering effects can result in incorrect findings when assessing source contribution.

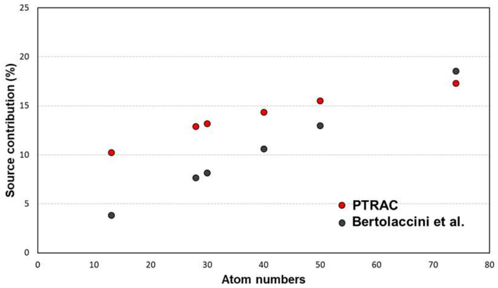

Fig. 3. Positron source contributions of a 7.6-μm Kapton foil

4. Conclusions

For PALS, the source contributions of the 7.6-um thick Kapton foil for the Al, Ni, Zn, Zr, Sn, and W samples were determined using the MCNP PTRAC function. The previous method underestimated the positron annihilation in the source-supporting foil by up to 62% compared to the Monte Carlo simulations. In conclusion, the source correction modeled by Monte Carlo simulations needs to be applied to PALS for accurate analysis of positron lifetime and relative intensities.

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