Geant4 simulation of the effect of backscattered positrons on the lifetime spectra of PLEPS

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Abstract. The Pulsed Low Energy Positron System (PLEPS) allows the measurement of positron lifetime spectra of very high quality with peak-to-background ratios up to \(3 \cdot 10^4\). At those peak-to-background ratios small structures appear in the lifetime spectra due to backscattered positrons. Despite their small overall contribution - less than 2% of the total events in the spectrum even with backscattering coefficient as high as 40% - those satellite structures can render the data analysis difficult. To understand the origin of those satellite structures and to further improve the performance of the system, comprehensive simulations of the target chamber of PLEPS have been undertaken. The results reproduce fairly well the background of the lifetime spectrum. It is now possible to identify the origin of the background structures and also plan some additional countermeasures.

1. Introduction
Positron Annihilation Lifetime Spectroscopy (PALS), when combined with a pulsed beam of variable energy, yields a very powerful technique capable of providing depth profiles of open volume defects e.g. in layered structures [1] and implanted samples [2] which are inhomogeneously damaged.

The Pulsed Low Energy Positron System [3] (PLEPS) at the high intensity positron source NEPOMUC [4] (NEutron-induced POsitron source MUnich) at the research reactor FRM-II is a user facility to perform high quality PALS measurements in very short times. Count rates up to \(10^4\) counts per second have been achieved, which results in short measuring time (about 10 minutes per lifetime spectrum with \(> 3 \cdot 10^6\) counts) and high peak to background ratios (up to \(3 \cdot 10^4\)). This allows routinely to separate up to four lifetimes.

New and ever more complicated layered materials require further improvements of the ability of PLEPS to separate more lifetimes. To this purpose two key factors have to be considered: a) time resolution and b) peak to background ratio.

(a) High time resolution is of particular importance for the separation of short–lived lifetime components. The time resolution of a pulsed positron beam is determined by the pulse width and the detector response. With small (<1 cm\(^3\)) scintillators, detector responses in the 100 ps range can be achieved. The trade off is a dramatic loss in event rate and consequently a high price to pay in terms of measurement time.

(b) High peak-to-background ratio with PLEPS may be achieved either by using two detectors face-to-face in coincidence or a single detector mounted immediately below the target.
Unfortunately the excellent peak-to-background ratio obtainable in the former case is out-weighted by the dramatic loss in event rate. For the single detector, at high peak-to-background ratios, structures due to backscattered positrons appear in the lifetime spectra. Already with the present setup the amount of events coming from backscattered positrons is less than 2% of the total counts in the lifetime spectrum even for high Z targets and high implantation energies (backscattering coefficient as high as 40%). These backscattered positrons partly increase the homogeneous background, whereas some cause satellite structures in the spectra (see figure 2). Note that even the most pronounced satellite structure contain less than 0.2% of the total counts in the lifetime peak. In spite of their small overall contribution, those satellite structures can render the analysis of the spectra difficult. Eliminating these satellite structures is presently the most promising way to improve the quality of the lifetime spectra and to augment the number of lifetimes, which can be separated with PLEPS. To this aim comprehensive simulations of the backscattered positrons in PLEPS have been performed.

2. Simulations

2.1. Electric and magnetic field modeling with COMSOL Multiphysics

PLEPS can be conceptually divided into two main parts: the pulsing section - consisting of a prebuncher, a chopper and a buncher operating at a frequency of 50 MHz, which corresponds to a time window of 20 ns - followed by the acceleration section - consisting of a drift tube, an accelerator and the target chamber. The target chamber consists of a Faraday cage and the sample holder, which is kept at the negative high voltage (0.5 kV - 20 kV). The potential of the Faraday cage is set to -2 kV with respect to the sample. This ensures that, in combination with the variable drift tube potential, the pulse shape is independent of the implantation energy and consequently the time resolution varies little over the full energy range. The positrons are magnetically guided through the system in a constant solenoidal field. For a detailed description of the entire system see [3]. In this work, we focus on positrons backscattered from the target. Therefore only the target chamber of PLEPS was considered. The electric and magnetic fields were determined by COMSOL Multiphysics [5].

The simulation of the magnetic field has been done using rotational symmetry and periodic boundary conditions. In figure 1 (a) the section of the target chamber parallel to the beam direction and the coils that generate the magnetic field are shown. The magnetic flux density is plotted as surface- and streamline-plots as a function of the position. The magnetic field is homogeneous along the beam path, except for the last 30 mm where the field increases due to the presence of the mu-metal shielding of the detector, and it is consistent with the measured values. In the Faraday cage the rotational symmetry is broken and, therefore, a three dimensional simulation of the electric field was necessary. The complicated fan-like structure of tungsten blades covered with Kapton in the top of the Faraday cage was replaced by a simple plate. Figure 1 (b) shows the section of the target chamber parallel to the beam direction, in which the electric potential as contour-plot and the electric field as arrow field are shown.

2.2. Simulation with Geant4 and results

With the electric and magnetic fields obtained by COMSOL, the trajectories of the backscattered positrons were simulated using Geant4 (release 9.5 patch 01) [6] and the PENEOLOPE (PENetration and Energy LOss of Positrons and Electrons and photons) low-energy electromagnetic model, including ionization, bremsstrahlung and multiple scattering. Geant4 takes into account the slowing down of the positrons inside the specimen. A range cut value of 1 nm and an energy threshold limit of 50 eV were set. To register only events that are actually seen by the detector, also the tungsten shielding of the detector was considered and the 511 keV annihilation quanta that deposited less than 300 keV were rejected like in the real experiment.
Figure 1. Section of the target chamber parallel to the beam direction showing the magnetic flux density as surface- and streamline-plots on the left side (a) and the electric potential as contour-plot and the electric field as arrow field on the right (b).

For each simulation $10^8$ positrons were implanted into the sample to obtain approximately the same number of events in the measured and in the simulated spectra. The annihilation position and the time between the implantation of the positron and the arrival of the gamma quantum in the detector were saved. We choose a gold target because due to its high backscattering coefficient the satellite structures are more pronounced than for other samples. The simulations have been performed for different positron implantation energies and the influence of the following possible countermeasures was studied: a) extending time window, b) using different materials in the top of the Faraday cage and c) varying the solenoidal magnetic field.

As an example, in figure 2 the comparisons between the measured spectra and the results obtained from the simulations at 4 keV positron implantation energy with time windows of 20 ns (left) and 40 ns (right) are shown for two different material in the top of the Faraday cage. From both the measured and the simulated spectra the constant background value was subtracted.

At 4 keV implantation energy (figure 2 (left)), the experimental measurement shows a very pronounced structures centered at 10 ns and a second one at the end of the time window and partly re-entering the time window from the opposite end. The simulation with tungsten in the top of the Faraday cage agrees very well with the experimental spectrum. Using a low Z material like Kapton instead of tungsten in the simulation, suppresses completely the folded structure under the lifetime peak.

Extending the time window (figure 2 (right)), independently of the material in the top of the Faraday cage, the fold-over of the second structure is completely avoided and this disturbance removed from the region under the peak of the lifetime spectrum and shifted to a position where the lifetime spectrum is already decayed. A first experimental test with a 40 ns time window has confirmed this result. The reduction of the second peak (centered at 22 ns) by using different materials could be of interest for samples with long lifetimes. At 4 keV implantation energy the
Figure 2. Measured lifetime spectrum of a gold target at 4 keV positron implantation energy and simulated background structure with two different materials in the top of the Faraday cage and time window of 20 ns (left) and of 40 ns (right).

influence of the magnetic field on the background structures was negligible. However, at higher implantation energies a small part of the backscattered positrons annihilates on the side walls of the target chamber and this results in a sharp structure centered at about 4 ns. Increasing the magnetic field in the target region prevents these positrons to annihilate on the side walls and thus allows to suppress this structure.

3. Conclusions

Comprehensive simulations of positrons backscattered from the sample and annihilating in the target chamber of PLEPS have been performed and compared to the measured lifetime spectra showing very good agreement. The simulations have shown three possible pathways to reduce the structures in the background: shifting the background structures outside the region of interest by a) extending the time window and b) increasing the magnetic field and c) reducing the backscattering coefficient of the top of the Faraday cage by using low Z materials.

Moreover, the possibility to almost quantitatively reproduce the behavior of backscattered positrons in the target chamber opens up a new way to check and determine the implantation profile on layered systems with depth-dependent Z-values by comparing the measured backscattered background as a function of the implantation energy with the simulated one.

Acknowledgment

Funding from the BMBF (Project 05K10WNA-Posimethod) is gratefully acknowledged.

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