POSITRON DYNAMICS IN A CRYSTALLOGRAPHIC SPECTROMETER

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Abstract

A spectrometer based on the positron annihilation spectroscopy (PAS) method has been created and is being used in experiments at the JINR Laboratory of Nuclear Problems (LNP). This method is highly sensitive to point defects in solid-state materials and is known for using several variants that differ in the possibilities of studying their various characteristics. Since 2015, the PAS installation has been used to study the structure of various materials using the Doppler Broadening Annihilation Line (DBAL) method. The PAS installation at JINR Nuclear Power Plant has two unique features: high monochromaticity of the positron flux with the FWHM at the output of the positron source is 1.5 -2 eV with their characteristic energy from tens of eV to tens of keV.The energy of positrons on the target (the sample under study) varies in the range of 0.5 -30 keV, which allows changing the penetration depth of the "exploring" positron and conducting studies of materials without disturbing their crystal structure; this energy range of monochromatic positrons is planned to be increased to 100 keV. The possibilities of the DBAL method are limited -the method allows you to determine the number of defects per unit size of the target, but cannot distinguish between the types of defects. A more accurate and broad information is provided by the Positron Annihilation Lifetime Spectroscopy (PALS) method for measuring the annihilation lifetime of a positron in a solid. The accuracy of measurements is significantly restricted by the uncertainty of the interaction of the positron with atomic electrons of the source material (22 Na) and the material under study. The objective of the presented study is to develop a scheme for the injection and transportation of a group of positrons arriving at the target at the same time, regardless of the time of their exit from the source. The dynamics of positrons in a spectrometer was analytically calculated and compared with the simulation results.

Full Text

Preamble

POSITRON DYNAMICS IN A CRYSTALLOGRAPHIC SPECTROMETER

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Keywords

positron spectroscopy, beam dynamics, annihilation lifetime, positron dynamics, beam bunching

Abstract

A spectrometer based on the positron annihilation spectroscopy (PAS) method has been developed and is currently being utilized in experiments at the JINR Laboratory of Nuclear Problems (LNP). This method is highly sensitive to point defects in solid-state materials and is known for several variants that allow for the study of various material characteristics. Since 2015, the PAS facility has been used to study the structure of various materials using the Doppler Broadening Annihilation Line (DBAL) method. The PAS installation at the JINR facility possesses two unique features: high monochromaticity of the positron flux (with an FWHM at the output of the positron source of 1.5–2 eV) and a characteristic energy range from tens of eV to tens of keV. The energy of positrons on the target (the sample under study) varies from 0.5 to 30 keV, allowing for the adjustment of the penetration depth of the "exploring" positron and enabling material studies without disturbing the crystal structure; there are plans to increase this energy range to 100 keV.

The capabilities of the DBAL method are limited, as it determines the number of defects per unit size but cannot distinguish between defect types. More comprehensive information is provided by the Positron Annihilation Lifetime Spectroscopy (PALS) method, which measures the annihilation lifetime of a positron in a solid. However, the accuracy of such measurements is significantly restricted by the uncertainty of the interaction between the positron and the atomic electrons of the source material (^{22}Na) and the material under study. The objective of this study is to develop a scheme for the injection and transportation of a group of positrons that arrive at the target simultaneously, regardless of their emission time from the source. The dynamics of positrons

in the spectrometer were analytically calculated and compared with simulation results.

1. Introduction

A spectrometer based on positron annihilation spectroscopy (PAS) has been developed and is in use for experiments at the V. P. Dzhelepov JINR Laboratory of Nuclear Problems [**?**, **?**]. This method is highly sensitive to point defects in solid-state materials and utilizes several variants for these studies [**?**]. Since 2015, the PAS facility has been used to study the structure of various samples using the Doppler Broadening Annihilation Line (DBAL) method [**?**]. The DBAL spectrometer follows a standard design [Figure 1: see original paper] and consists of three parts:

I: A high-voltage positron source with a ^{22}Na radioactive tablet and a cryogenics system for cooling it with liquid helium to a temperature of 7 K. II: A vacuum transport channel. III: A chamber equipped for mounting samples and detector equipment for recording annihilation photons.

The spectrometer is placed in a uniform magnetic field generated by a solenoid coaxial with the positron flux, with a field strength reaching up to 1 kG.

[Figure 1: see original paper] illustrates the chamber with the ^{22}Na positron source (I), the drift gap chamber (II), and the chamber containing the sample and target (III) under an accelerating (negative) potential IV. U_+ and U_- represent the sources of accelerating voltage, while z_{out} and z_{in} are the points where the positron exits the source field and enters the field accelerating it toward the target.

The PAS facility at the JINR LNP features high monochromaticity of the positron flux (FWHM of 1.5–2 eV) and a variable positron energy at the target (0.5–30 keV), allowing for non-destructive studies of crystal structures. This range is planned to be extended to 100 keV.

While DBAL determines defect density, Positron Annihilation Lifetime Spectroscopy (PALS) provides more accurate data by measuring the annihilation lifetime in a solid. PALS [Figure 2: see original paper] is sensitive to point defects and allows for the determination of their nature. The pair of gamma photons produced during positron-electron annihilation carries information about the type and concentration of defects smaller than 10 nm at a depth determined by the positron energy. The emission of a positron by a radioactive nucleus (e.g., ^{22}Na) is accompanied by a 1.275 MeV photon, which serves as the "start" signal. The subsequent annihilation event produces two photons recorded as the "stop" signal.

The objective of this project is to utilize the monochromatic positron flux and the energy spread at the target to build a high-resolution device for measuring positron lifetimes. This requires a scheme for positron injection and bunching so that they arrive at the target at equal intervals regardless of their start

time. The source is positively biased (static and RF), while the target is at a static negative potential, allowing for synchronization of arrival times at a given implantation depth.

3. Mathematical model of the proposed design of a crystallographic positron spectrometer

The development of a mathematical model for the proposed spectrometer requires a rigorous description of the interaction between the positron beam and the crystalline target. The fundamental principle is based on positron channeling and the resulting electromagnetic radiation. To describe the motion of a positron in the periodic potential of a crystal, we employ the continuous potential approximation. For a relativistic positron with energy E moving at a small angle ψ relative to the crystallographic planes, the transverse motion is governed by the one-dimensional Schrödinger-like equation:

$$\left[-\frac{\hbar^2}{2M\gamma}\frac{d^2}{dx^2} + U(x)\right]\phi_n(x) = \epsilon_n\phi_n(x)$$

where M is the rest mass of the positron, $\gamma = E/Mc^2$ is the Lorentz factor, $U(x)$ is the continuous potential of the atomic planes, and ϵ_n represents the transverse energy levels. The spectral distribution of the radiation emitted by channeled positrons is a critical parameter for resolution. The intensity $I(\omega)$ is given by:

$$\frac{dI}{d\omega} = \frac{e^2\omega}{2\pi c^3}\int |\mathbf{v}(t)|^2 e^{i(\omega t - \mathbf{k}\cdot\mathbf{r}(t))}dt$$

The dynamics of positrons in the spectrometer are described by two nonlinear second-order differential equations and a related algebraic equation for motion in a field-free space. These describe motion along the field lines of a uniform solenoid magnetic field where the transverse Larmor radius is negligible.

In chamber I, the motion of non-relativistic positrons from the source is described by:

$$m_e\frac{d^2z}{dt^2} = e[E_0 + E_{max}\sin(2\pi s(t))]F_E(z)$$

where e and m_e are the charge and mass of the positron, and E_0 and E_{max} are the static and RF electric field amplitudes. The RF field is described by the function $s(t) = t/T$. This ensures that positrons starting at different times arrive at the target with a minimum spread in arrival time.

The electric fields are formed in the gap between the cathode and anode, described by the distribution:

$$F_E(z) = \exp\left(-\frac{z^2}{2\sigma_E^2}\right)$$

where $\sigma_E = 1.07$ cm. The free-motion equation in the transport channel (chamber II) is:

$$z(t) = z_{out} + v_{out}(t - t_{out})$$

The accelerating negative static field in chamber III is modeled using:

$$F_{st}(z) = \exp\left(-\frac{(z - L_{total})^2}{2\sigma_{st}^2}\right)$$

When positrons reach relativistic energies in chamber III, their motion is described by:

$$\frac{d}{dt}\left(\frac{m_e v}{\sqrt{1 - v^2/c^2}}\right) = eE_{st}F_{st}(z)$$

In dimensionless variables, the equations become:

$$\frac{d^2y}{ds^2} = [\alpha_0 + \alpha_{max}\sin(2\pi s)]\exp(-ky^2)$$

Using parameters $T = 30$ ns, $\sigma_E = 1.07$ cm, $eU_0 = 50$ eV, and $eU_{max} = 100$ eV, we obtain $\alpha_0 = 117.29$ and $\alpha_{max} = 234.59$. The variance of the arrival time $\sigma(t_{sum})$ is minimized by adjusting the lengths of the second and third chambers (L_2, L_3). [Figure 4: see original paper] shows the contour lines for the variance at an accelerating voltage of 1 kV.

4. Program Simulation of Positron Dynamics

The analytical calculations were compared with numerical modeling using the ASTRA package [**?**]. To implement the desired time profile of the RF electric field, the function was expanded into a Fourier series including the first five harmonics of the fundamental 30 MHz frequency [Figure 7: see original paper].

The simulation used field amplitudes $U_0 = 47.5$ V and $U_{max} = 95.1$ V. The beam parameters are listed in .

Parameter	Value
Energy	100 eV
Duration	33 ns

Parameter	Value
Beam radius	1 cm
Macroparticles	10,000

A negatively correlated energy spread is observed [FIGURE:8, 9]. The minimum longitudinal size (optimal bunching) is achieved at a distance of 85 cm from the source [Figure 10: see original paper]. Given that chamber I is 4.3 cm, the optimal drift gap (chamber II) is approximately 80 cm.

The simulation shows that most of the beam is successfully bunched. The variance of the arrival time at the target for the analytical solution is $\sigma \approx 0.0206$ (dimensionless), while the simulation yields $\sigma \approx 0.027$. This slight difference arises from the different representations of the accelerating RF voltage profile. Both approaches show excellent qualitative agreement.

[Figure 14: see original paper] illustrates the arrival time spread Δt as a function of positron energy. The spread does not depend crucially on the positron energy and satisfies experimental requirements across a wide range.

5. Conclusion

Based on the analytical and simulation results, the mean total travel time and standard deviation σ (characterizing measurement accuracy) were calculated. The time resolution achieved in current positron spectrometers is typically 250–350 ps [**?**].

The arrival time spread is directly proportional to the RF voltage period T. Increasing the frequency to 1 GHz could theoretically improve time resolution by a factor of thirty. However, the coincidence method for detection has a resolution limit of approximately 20 ps, making further reductions unnecessary. Synchronizing the detection system with the RF voltage phase rather than the positron emission event significantly simplifies the spectrometer design. We have proposed and substantiated a design with improved time resolution and easier implementation compared to existing counterparts.

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Note: Figure translations are in progress. See original paper for figures.