Positron Annihilation Techniques for Defect Structure Analysis in Irradiated Ceramic and Nanocrystalline Materials

1. Introduction:

The investigation of defects in the structure of advanced materials such as ceramics, nanocrystals, polymers, thin films, and semiconductors has garnered significant scientific interest due to their crucial role in determining the physical, chemical, electrical, and mechanical properties of these materials. In particular, the presence, type, and concentration of defects — including vacancies, interstitials, and dislocations — critically influence charge transport, optical transparency, magnetic behavior, and structural stability, which are essential parameters for applications in microelectronics, photonics, sensors, and energy devices.

In recent decades, increasing attention has been paid to understanding how radiation — including gamma rays, protons, and neutrons — affects the defect structure of solid-state materials. Under irradiation, atoms are displaced from their lattice positions, leading to the formation of point defects, vacancy clusters, dislocation loops, and amorphous zones. These radiation-induced defects can modify mechanical resilience, conductivity, and diffusion properties and thus play a crucial role in the material's long-term reliability, particularly in nuclear, aerospace, and semiconductor industries. Understanding the mechanisms of defect formation and evolution under different radiation doses and annealing conditions is therefore a prerequisite for designing radiation-tolerant materials.

Positron Annihilation Lifetime Spectroscopy (PALS) and Doppler Broadening Annihilation Spectroscopy (DBAS) have emerged as highly sensitive and non-destructive techniques for probing open-volume defects and characterizing their nature and concentration. PALS is particularly effective in quantifying the size and density of vacancy-type defects by measuring the positron lifetime components, which correlate with the local electron density. DBAS, on the other hand, provides information about the chemical environment and momentum distribution of the electrons at the annihilation site through the analysis of S and W parameters. The complementary use of these positron annihilation techniques enables a comprehensive understanding of defect evolution, especially in irradiated materials, where conventional methods often fall short due to limited resolution or destructive sample preparation.

2. Main part:

Participant:

- To acquire knowledge about positron annihilation techniques for material characterization;
- To learn the principles of defect identification and positron trapping models;
- To understand how irradiation and annealing affect materials;
- To process experimental PALS and DBS data;
- To perform comparative analysis of results for materials exposed to different radiation conditions.

3. Description of work on the project

3.1. Experimental Setup:

Positron Annihilation Lifetime Spectroscopy

A fast positron lifetime spectrometer equipped with two BaF_2 scintillators and a time resolution of 250 ps (as determined by the full width at half maximum, FWHM) is used to determine the lifetime components in PALS studies of the samples. The positron source used in the measurements is a ^{22}Na isotope with an activity of 10.5 μCi. The source is encapsulated between titanium foils with a thickness of 7 μm. It is placed in a "sandwich" configuration between two identical samples. Approximately 15% of the emitted positrons annihilate within the source with lifetimes of 254 ps (96%) and 1.2 ns (4%). During analysis, background and source contributions must be subtracted. In the experiments, positron lifetime spectra should be acquired over 24 hours with the collection of more than ~2–3 × 10^6 events. The data are analyzed using the LT 9.2 software package to determine the lifetime components and their relative intensities. Figure 1 presents a schematic and schematic description of the PALS equipment.

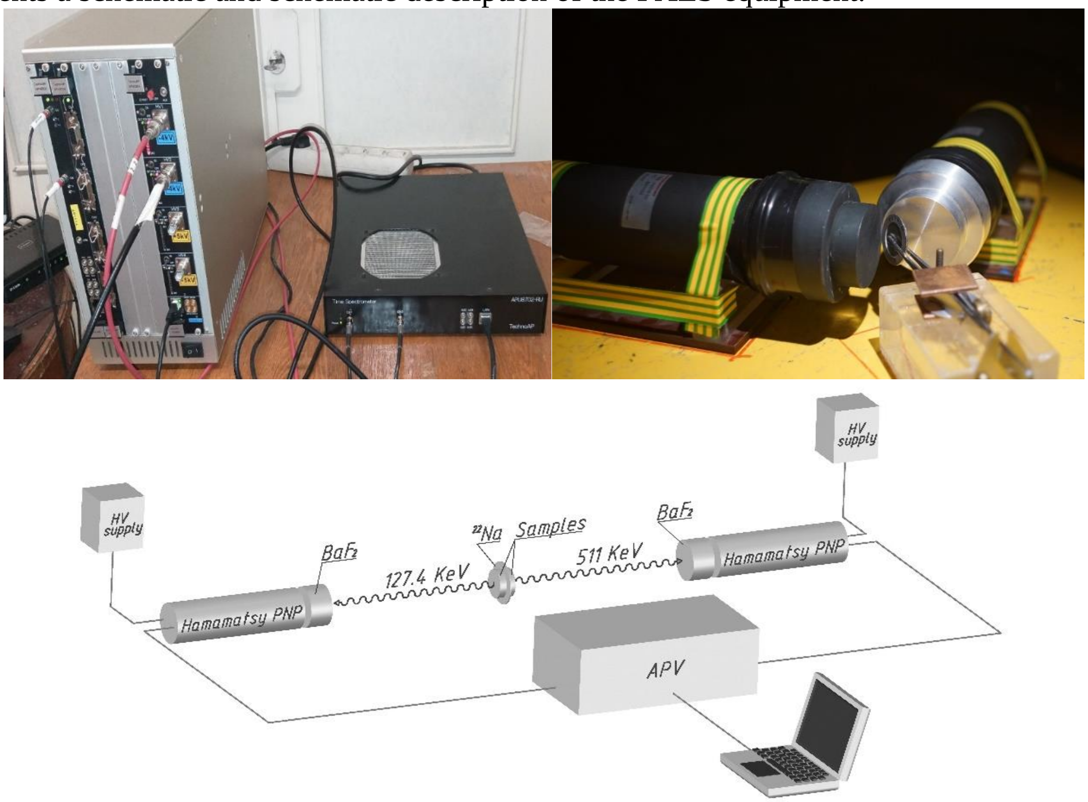

Fig. 1. Description of PALS equipment and scheme

Doppler Broadening Annihilation Spectroscopy

In Doppler Broadening studies, a high-purity germanium (HpGe) detector cooled with liquid nitrogen and having an energy resolution of 1.2 keV at 511 keV is used. The positron source consists of a ^{22}Na isotope with an activity of approximately 20 mCi and a positron emission intensity of 10^5 e^+/s. The investigations are carried out under high vacuum conditions of about 10^{-9} Torr. Analysis of the obtained DBS spectra yields the S and W parameters. The S parameter represents the ratio of the area of the central part of the spectrum to the total area, while the W parameter corresponds to the ratio of the wing areas (both sides) of the spectrum to the total area (see Figure 2).

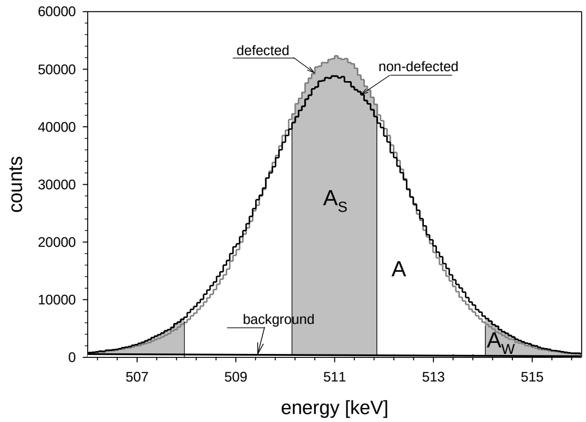

Fig. 2.

The SP-SE and SigmaPlot software packages are used for the analysis of the DBS data sets. The following image shows a complete description of DBAS. Figure 3 depicts a complete view of DB spectroscopy.

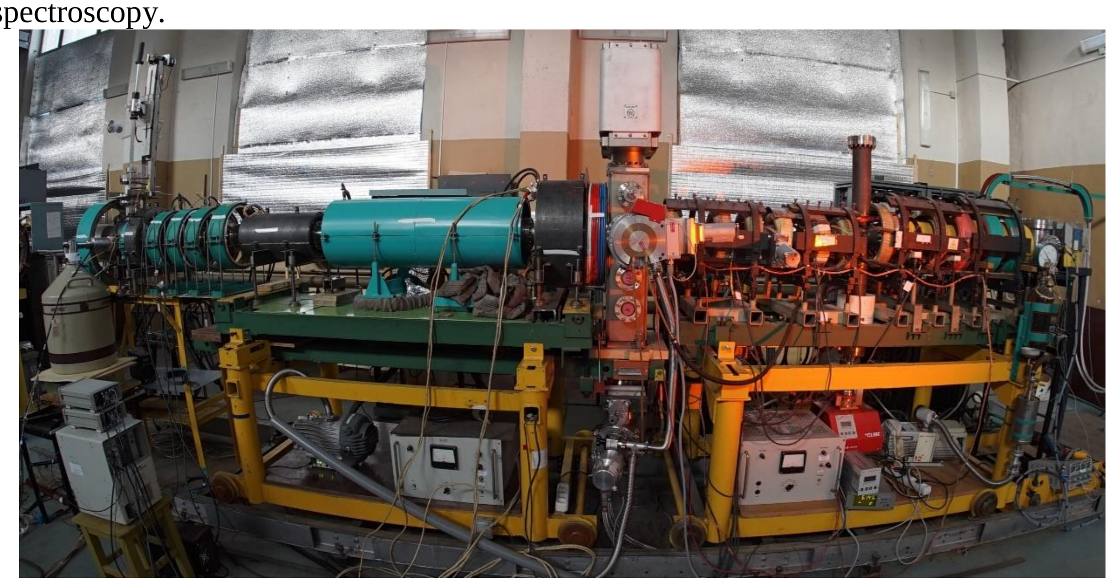

Fig. 3. Complete view of DB spectroscopy

3.2. Measurement Procedure:

- Preparation of samples for PALS and DBAS studies;
- Calibration of the lifetime spectrometer using Standard References in PALS studies;
- Preparation of samples for DBAS studies and participation in studies;
- Mastering and implementation of SP-SE, VEPFIT program codes used for DBAS data analysis;
- Discussion of the results and preparation for writing the article;

3.3. Presentation of results:

- Preparation of a FINAL REPORT ON RESULTS for JINR, with the results being authored by the participating studentPreparation of a FINAL REPORT ON RESULTS for JINR

4. Requirements for the level of student preparation.

- Basic knowledge of solid-state physics or materials science;
- Familiarity with radiation physics and spectroscopy is desirable;
- Skills in data processing are advantageous;
- Minimal knowledge of charged particle dynamics;

5. Recommended literature in English.

1) Home page - Jerzy Dryzek - Research
2) R Krause-Rehberg, HS Leipner, Positron annihilation in semiconductors: defect studies, Springer Science & Business Media (1999).
3) S.F. Samadov, N.V.M. Trung, A.A. Donkov, A.A. Sidorin, O.S. Orlov, E. Demir, O.A. Samedov, S.H. Jabarov, N.V. Tiep, E.P. Popov, M.N. Mirzayev, Investigating the impact of gamma irradiation and temperature on vacancy formation and recombination in ZrB_2 ceramics using positron annihilation spectroscopy, Journal of Nuclear Materials. 599 (2024) 155242, https://doi.org/10.1016/j.jnucmat.2024.155.
4) Kansy J., 1996. Microcomputer program for analysis of positron annihilation lifetime spectra. Nucl. Inst. Meth. Phys.ics Res. 374 (2), 235-244. https://doi.org/10.1016/0168-9002(96)00075-7.
5) Selim F.A., 2021. Positron annihilation spectroscopy of defects in nuclear and irradiated materials-a review. Mater. Charact. 174, 110952. https://doi.org/10.1016/j.matchar.2021.110952.
6) F. Tuomisto, I. Makkonen, Defect identification in semiconductors with positron annihilation: Experiment and theory, Rev. Mod. Phys. 85 (2013), https://doi.org/10.1103/RevModPhys.85.1583.
7) P. Horodek, K. Siemek, Positron Beam Characteristics of Heavy Ion Irradiated Silver, Acta Phys. Pol. A. 142 (2023) 697-701, https://doi.org/10.12693/APhysPolA.142.697.

6. Number of project participants:

The project is intended for a student working individually.

7. Project Manager from JINR:

Dr. Samir Samadov PhD,

Senior Researcher, Laboratory of Nuclear Problems (LNP), JINR

Scientific Interests: Radiation effects in materials, positron annihilation spectroscopy, defect physics