



**15th International Workshop on Slow Positron Beam
Techniques and Applications (SLOPOS-15)**

Book of Abstracts

BOOK OF ABSTRACTS

15th International Workshop on Slow Positron Beam Techniques and Applications (SLOPOS-15)

Prague September 2-6, 2019

Faculty of Mathematics and Physics, Charles University
Malostranské náměstí 2/25, 181 00 Praha 1, Czech Republic



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SLOPOS-15 Programme

PL – plenary lecture (35+5 min), IT – invited talk (25+5 min), T – talk (15+5 min), P – poster.

Monday, September 2, 2019		
7:00 – 8:00	Registration. Coffee & breakfast.	
8:00 – 8:20	Opening.	
8:00 – 8:10	Ladislav Skrbek , Vice-dean, <i>Faculty of Mathematics and Physics, Charles University, Czech Republic</i> : Opening of SLOPOS-15.	
8:10 – 8:20	Organization remarks.	
8:20 – 10:30	Positron surface science.	Pg.
PL-1 8:20 – 9:00	Alex H. Weiss , <i>The University of Texas at Arlington, USA</i> : Novel Positron Annihilation Based Surface Spectroscopies	12
IT-1 9:00 – 9:30	Ken Wada , <i>National Institutes for Quantum and Radiological Science and Technology, Takasaki, Japan</i> : A low-energy positron diffraction (LEPD) experiment station for a linac-based slow-positron beam.	13
IT-2 9:30 – 10:00	Izumi Mochizuki , <i>Institute of Materials Structure Science, KEK, Japan</i> : Recent Studies of Surface Structure Analysis with Total-Reflection High-Energy Positron Diffraction (TRHEPD) at Slow-Positron Facility, KEK.	14
IT-3 10:00 – 10:30	Kenji Ito , <i>National Institute of Advanced Industrial Science and Technology (AIST), Japan</i> : Na-22 based low-energy AMOC measurements for chemical analysis of the free-volume holes in hydrocarbon-silica hybrid thin films.	15
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11:00 – 12:50	Ps physics and Ps beams.	Pg.
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IT-4 11:40 – 12:10	Sebastiano Mariazzi , <i>University of Trento, Italy</i> : Techniques for production and detection of a 2^3S positronium beam.	17
T-1 12:10 – 12:30	Ross E. Sheldon , <i>University Colledge London, UK</i> : A Multi-ring Electrostatic Guide for Rydberg Positronium.	18
T-2 12:30 – 12:50	Lokesh Gurung , <i>University Colledge London, UK</i> : Precision microwave spectroscopy of the $n=2$ positronium fine structure.	19
12:50 – 13:00	Conference photo.	
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T-3 14:00 – 14:20	Akira Ishida , <i>The University of Tokyo, Japan</i> : Recent progress towards positronium Bose-Einstein condensation.	20

T-4 14:20 – 14:40	Nikodem Krawczyk , <i>Jagiellonian University, Krakow, Poland</i> : Studies of quantum entanglement in positronium decay with the J-PET detector.	21
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T-6 15:00 – 15:20	Aleksander Gajos , <i>Jagiellonian University, Krakow, Poland</i> : Studies of ortho-positronium decays into three photons with the J-PET detector.	23
T-7 15:20 – 15:40	Jyoti Chhokar , <i>Jagiellonian University, Krakow, Poland</i> : Charge symmetry test in decays of positronium atoms using the J-PET detector.	24
T-8 15:40 – 16:00	Sushil Sharma , <i>Jagiellonian University, Krakow, Poland</i> : TOT method for the disentanglement of photons in Positron Annihilation Lifetime Spectroscopy.	25
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16:30 – 18:30	Ps in solids & liquids.	Pg.
IT-5 16:30 – 17:00	Roberto S. Brusa , <i>University of Trento, Italy</i> : Open volumes structure and molecular transport in polymer and biopolymer nanocomposites.	26
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T-10 17:50 – 18:10	Bożena Zgardzińska , <i>Maria Curie-Skłodowska University, Lublin, Poland</i> : INTI plot – a new standard for the presentation of PALS results.	29
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IT-7 8:40 – 9:10	Akira Uedono , <i>University of Tsukuba, Japan</i> : Annealing behaviours of open spaces in thin Al ₂ O ₃ films deposited on semiconductors studied using monoenergetic positron beams.	32
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T-14 9:50 – 10:10	Francesco Guatieri , <i>Forschungs-Neutronenquelle, Heinz Maier-Leibnitz (FRM-II), Garching, Germany</i> : Simulating positron to positronium conversion in nanostructured materials.	35
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T-18 12:40 – 13:00	Yanyun Ma , <i>National University of Defence Technology, Changsha, China</i> : Generation of quasi-monoenergetic high energy positrons based on laser wakefield accelerated electrons.	41
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T-20 15:20 – 15:40	Shoji Ishibashi , <i>National Institute of Advanced Industrial Science and Technology (AIST), Japan</i> : Calculation of positron states and annihilation parameters in gamma and amorphous Al ₂ O ₃ .	45
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16:30 – 18:00	Development of positron beams & techniques.	Pg.
IT-12 16:30 – 17:00	Koji Michishio , <i>National Institute of Advanced Industrial Science and Technology (AIST), Japan</i> : Current status of the AIST slow positron facility.	47
T-22 17:00 – 17:20	Lukasz Kaplon , <i>Jagiellonian University, Krakow, Poland</i> : Development of Fast Plastic Scintillators for Positron Annihilation Lifetime Spectroscopy.	48
T-23 17:20 – 17:40	Jerzy Dryzek , <i>Institute of Nuclear Physics PAN, Krakow, Poland</i> : On the reconstruction of defect depth profiles obtained from the positron annihilation experiment and chemical etching.	49
T-24 17:40 – 18:00	Valerio Toso , <i>Politecnico di Milano, Italy</i> : Sensitivity of nuclear emulsions to low-energy positrons.	50
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20:00 – 22:00	Evening excursion to <i>Prague's castle</i> .	

Wednesday, September 4, 2019

8:00 – 10:30	Development of positron beams & techniques.	Pg.
PL-4 8:00 – 8:40	Christoph Hugenschmidt , <i>Technische Universität München, Garching, Germany</i> : Determination of the Vacancy Formation Enthalpy Revisited by Temperature Dependent Doppler-Broadening Spectroscopy.	51
IT-13 8:40 – 9:10	Werner Egger , <i>Universität der Bundeswehr München, Germany</i> : The pulsed low energy positron system PLEPS: applications and new developments.	52
T-25 9:10 – 9:30	Matthias Dodenhöft , <i>Heinz Maier-Leibnitz Center (MLZ) and Technische Universität München (TUM), Germany</i> : Total Reflection High-Energy Positron Diffractometer at NEPOMUC.	53
T-26 9:30 – 9:50	Marcel Dickmann , <i>Universität der Bundeswehr München, Germany</i> : Upgrade of the NEPOMUC re-moderator.	54
T-27 9:50 – 10:10	Eric Hirschmann , <i>Helmholtz-Zentrum Dresden-Rossendorf, Germany</i> : Digital positron lifetime spectroscopy for applications with high count rates.	55
T-28 10:10 – 10:30	Laurent Weber , <i>Teledyne SP Devices, Geneva, Switzerland</i> : Optimized High-speed digitizers for slow positron applications.	56
10:30 – 11:00	Coffee break.	
11:00 – 13:20	Development of positron beams & techniques.	Pg.
IT-14 11:00 – 11:30	Maik Butterling , <i>Helmholtz-Zentrum Dresden-Rossendorf, Germany</i> : Status of the Positron Sources at the Superconducting Electron LINAC ELBE.	57
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T-29 12:00 – 12:20	Andreas Wagner , <i>Helmholtz-Zentrum Dresden-Rossendorf, Germany</i> : Do we need a mono-energetic spin-polarized positron beam?	59
T-30 12:20 – 12:40	Yingjie Wang , <i>Institution of High Energy Physics and University of Chinese Academy of Sciences, Beijing, China</i> : Positron burst detecting array system based on SiPM and DRS4.	60
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IT-16 8:00 – 8:30	Stephan W.H. Eijt , <i>TU Delft, The Netherlands</i> : The role of vacancies and hydrogen in the photochromism of YO_xH_y thin films examined by in-situ Positron Annihilation Spectroscopy and μ SR.	62
IT-17 8:30 – 9:00	David Keeble , <i>University of Dundee, UK</i> : Variable energy positron annihilation lifetime spectroscopy studies of perovskite oxide electronic materials.	63
IT-18 9:00 – 9:30	Kelvin G. Lynn , <i>Washington State University, Pullman, USA</i> : Positron Annihilation studies of Various doped β - Ga_2O_3 Single Crystals with a Variable Energy Positron Beam.	64
T-32 9:30 – 9:50	Shigeru Yoshimoto , <i>Toray Research Center, Inc., Shiga, Japan</i> : Depth-resolved porosity of subnanoporous silica films elucidated by the low-energy positron lifetime technique and in-situ FT-IR-ATR.	65
T-33 9:50 – 10:10	Jonathan Slotte , <i>Aalto University, Finland</i> : Compensating defects in epitaxial Ge and Ge_xSn_{1-x} .	66
T-34 10:10 – 10:30	Nikolay Arutyunov , <i>IPLT (Institute of Electronics), Tashkent, Uzbekistan</i> : Positron annihilation in polyelectron system of strong spin-orbit field induced by bismuth impurity centers in natural silicon.	67
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T-35 11:30 – 11:50	Ahmed G. Attallah , <i>Helmholtz-Zentrum Dresden-Rossendorf, Germany</i> : Different curing strategies to create isolated pores in ultra-low-k thin films.	69

T-36 11:50 – 12:10	Jacques Botsoa , <i>CNRS, CEMHTI, Université d'Orléans, France</i> : The origin of p-type conductivity in thin films of copper chromium delafossites deposited by Metal-Organic Chemical Vapor deposition investigated by Positron Annihilation Spectroscopy.	70
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13:00 – 14:00	Lunch, restaurant Profesní dům (base floor of the conference venue).	
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T-39 14:30 – 14:50	Laura Resch , <i>Institute of Materials Physics, Graz University of Technology, Austria</i> : Artificial Aging of a Commercial Light Weight Alloy Studied by In-situ Positron Beam Doppler Broadening Spectroscopy.	74
T-40 14:50 – 15:10	Alaaeldin M. Ibrahim , <i>Martin-Luther University, Halle, Germany</i> : Effect of trace elements and quenched-in vacancies on precipitation hardening in Al-1.7at%Cu alloy.	75
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T-44 17:30 – 17:50	Ewelina Kubicz , <i>Jagiellonian University, Krakow, Poland</i> : Studies of alive normal and cancer cell lines and tissues in vitro with Positron Annihilation Lifetime Spectroscopy.	80
19:00 – 23:00	Banquet at the Assembly hall of the Lesser Town Palace.	
Friday, September 6, 2019		

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IT-22 8:40 – 9:10	Atsuo Kawasuso , <i>National Institutes for Quantum and Radiological Science and Technology, Takasaki, Japan</i> . Positronium Formation at Metal, Semiconductor and Graphene Surfaces.	82
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T-50 12:20 – 12:40	Anna Macková , <i>Nuclear Physics Institute of the Czech Academy of Sciences, Řež, Czech Republic</i> : Ion beam modification of crystalline materials for optoelectronic application.	90
13:00 – 14:00	Lunch, restaurant Profesní dům (base floor of the conference venue).	
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14:00 – 14:20	Summary of SLOPOS-15.	
14:20 – 14:30	Closing remarks.	
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Poster session (Tuesday, September 3, 2019, 18:00 – 20:00)		Pg.
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P-3	Baoyi Wang , <i>Institution of High Energy Physics and University of Chinese Academy of Sciences, Beijing, China</i> : Measurement of annihilation lifetime for positron burst.	93
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Novel Positron Annihilation Based Surface Spectroscopies

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Recent results will be reviewed which demonstrate how positron based surface spectroscopies can obtain information regarding surface phenomena that are unobtainable by other techniques. Positron annihilation induced Auger electron emission, first reported in 1988, forms the basis of a top-layer specific surface spectroscopy, Positron Annihilation Induced Auger Electron Spectroscopy (PAES) [1]. The high degree of surface specificity of PAES results from the trapping of the positron in an image potential well just outside the surface prior to the annihilation of the positron with a core or deeply bound valence electron. Chemical information regarding the surface is obtained from an analysis of the energy of electrons emitted as a result of the filling of the annihilation induced hole through an Auger transition. Furthermore, the use of low energy positrons (< 1.5 eV) allows PAES to measure Auger electrons down to 0 eV without any secondary electron background. We have recently used the high surface selectivity and background free nature of PAES to measure the Auger spectra (0 eV to 600 eV) from graphene over layers that are only a few layers (1-8) thick [2]. Recently it has been proposed [3] to take advantage of the localization of the positron at surfaces to obtain top-layer specific surface information from an analysis of the Doppler broadened gamma spectra. Here we report preliminary results obtained using both gamma-gamma and gamma-Auger electron coincidence that provide evidence that Doppler broadened annihilation gamma spectroscopy could be applied to surface analysis and that such a spectroscopy could be used to characterize both external and internal surfaces under in-situ (operando) conditions.

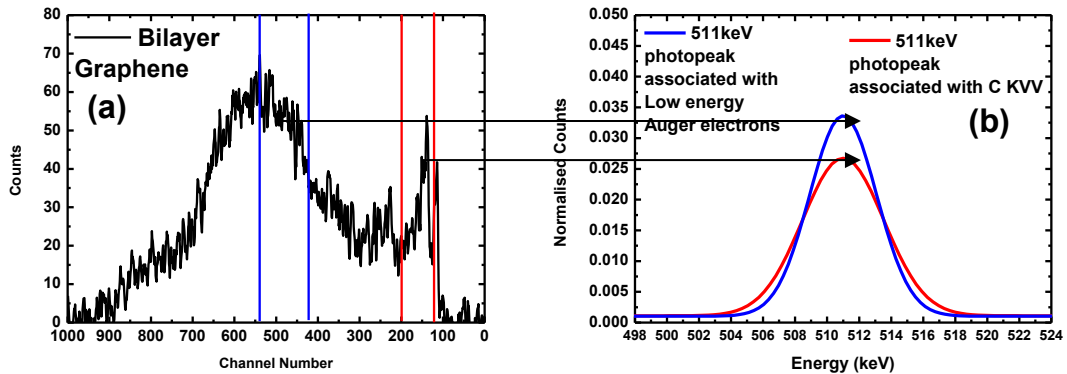


Figure 1 Panel (a) shows time of flight PAES data from Graphene. We interpret the intensity in the regions between the coloured lines as due to Auger electron emission resulting from annihilation-induced holes in the C 1s level (red lines) and in the graphene valence band and O 2s level (blue lines). Panel (b) shows a comparison of the Doppler broadened gamma spectra obtained in coincidence with Auger electrons in the corresponding regions.

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A low-energy positron diffraction (LEPD) experiment station for a linac-based slow-positron beam

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Low-energy positron diffraction (LEPD), which is the positron counterpart of low-energy electron diffraction (LEED), has been evaluated by a LEED theorist as an ideal surface structure analysis method [1]. In 1979, the first LEPD was observed by the Brandeis Univ. group with a channel electron multiplier using a slow-positron beam from a radioisotope (RI) source [2]. Subsequently they developed a system for observing a LEPD pattern with multiple spots and demonstrated that LEPD experimental results are more closely reproduced by a dynamical diffraction theory than in LEED [3]. Unfortunately, however, LEPD experimental research has been discontinued for about last two decades because of the difficulty in obtaining a low-energy positron beam with sufficient intensity and quality.

We have utilized a high-intensity slow-positron beam generated by a linear-electron-accelerator (linac) and succeeded in observing diffraction patterns of a Ge(001)-2×1 surface structure [4]. This is the first LEPD observation with a linac-based slow-positron beam and expected to open the way to provide a fundamental tool for surface structure analysis along with total-reflection high-energy positron diffraction (TRHEPD) [5].

There are a number of differences between an RI-based LEPD system and a linac-based one. One difference is the time structure of the beam. While an RI-based system provides a continuous beam, a slow-positron beam generated with a normal-conducting linac has a pulsed time-structure reflecting that of the linac beam. A high-intensity pulsed slow-positron beam could cause a multi-hit problem in the detection system with a position sensitive detector. To address this problem, a pulse stretcher for ~ 5 keV beam with an approximately 6-m long Penning-Malmberg trap has been developed [4].

Another difference is the beam transportation methods. The RI-based LEPD system employed electrostatic lenses along the whole beam-line, while linac-based systems transport the beam from a remote positron production unit along the beam-line with a magnetic field. A transmission-type brightness-enhancement system with a 150-nm-thick Ni foil and electrostatic optics have been developed to allow low-energy positron beams interacting with a sample in a non-magnetic field region with a sufficient beam intensity and quality.

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Recent Studies of Surface Structure Analysis with Total-Reflection High-Energy Positron Diffraction (TRHEPD) at Slow-Positron Facility, KEK

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Total-reflection high-energy positron diffraction (TRHEPD) [1, 2] is the positron counterpart of reflection high-energy electron diffraction (RHEED). It provides an ideal technique for the determination of the topmost and the subsurface structure of a crystal [1-5].

Recent results of the surface structure determination performed by using the TRHEPD apparatus at the Slow-Positron Facility (SPF) [6], IMSS, KEK, are reported. The facility provides a linac-based intense energy-tuneable positron beam. A brightness-enhancement system [7] enables acquisition of a clear TRHEPD pattern within a practical measurement timeframe.

The detailed coordinates of the germanene atoms on an Al (111) surface was experimentally determined [8]. It unveiled that the germanene has an asymmetric buckling unlike the models previously reported. The structure of superconducting Ca-intercalated bilayer graphene on a SiC (0001) surface was determined. It made clear the relation between the atomic arrangement and the superconductivity in the Ca-intercalated graphene [9]. The azimuthal-plots analysis, which was proposed for RHEED before [10], is applied to THREPD [11] as a method to make full use of exceeding surface sensitivity of the positron. Its performance is examined with rutile-TiO₂ (110) (1×1) surface of which the atomic arrangement is well-established.

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Na-22 based low-energy AMOC measurements for chemical analysis of the free-volume holes in hydrocarbon-silica hybrid thin films

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Our group has so far proved that the positron and positronium (Ps) momentum distributions for polymers associate with their constituent elements [1,2], indicating that Ps is also useful for probing the chemistry of free-volume surfaces. The chemical environment from a nanoscopic viewpoint has been investigated for bulk polymers by means of the positron age-momentum correlation (AMOC) technique, which demonstrated the applicability of AMOC to chemical analysis around the free volumes [3]. In the present work, an energy-tunable AMOC measurement system with a Na-22-based pulsed positron beam was developed for investigating functional thin materials (Figure) [4]. Results of AMOC measurements using the developed system for hydrocarbon-silica hybrid thin films, fabricated through plasma-enhanced chemical vapor deposition [5], are demonstrated, and the effect of the decomposition of the hydrocarbon components on the free-volume structure is discussed based on the obtained AMOC data.

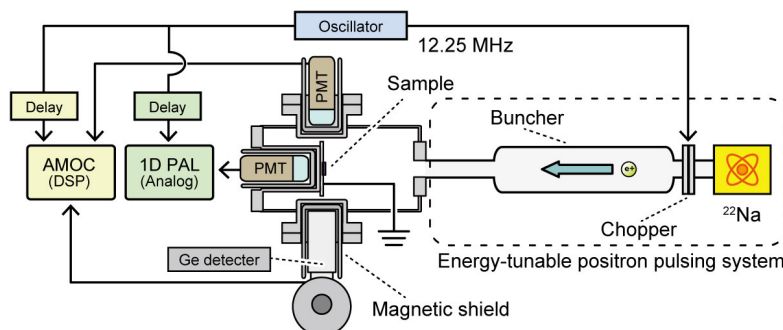


Figure: Schematics of the developed low-energy AMOC system Ref. [3].

This work was achieved with tremendous help of technical suggestions and continuous encouragements from the AIST positron team as follows; Dr. Yoshinori Kobayashi, Dr. Ryoichi Suzuki, Dr. Nagayasu Oshima, Dr. Brian O'Rourke, Dr. Hideaki Hagihara, and Dr. Hiroshi Yanagishita. Technical support from TechnoAP and FUJI IMVAC for the construction of the AMOC system is acknowledged. This work was supported by JSPS KAKENHI Grant Number 16H04526.

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Recent experimental progress in positronium-laser physics

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The field of experimental positronium physics has advanced significantly in recent years, in many cases by employing new techniques for trapping and manipulating positrons using Surko-type buffer gas traps [1]. These devices capture and store positrons, allowing for the production of high quality DC beams, or high intensity pulsed beams. The latter approach can be used to create an instantaneous cloud of Ps atoms that can be probed with standard ns pulsed lasers. This allows for the optical production of excited Ps states, ranging from 2P levels, which decay back to the ground state in 3.2 ns, to metastable 2S states, that cannot decay radiatively, but will self-annihilate (in 1.1 microseconds), to long-lived Rydberg states, that do not annihilate at all and, for easily produced states, may have radiative lifetimes of hundreds of microseconds [2]. The ability to generate Ps atoms in excited states facilitates numerous experimental programs [3], including precision optical and microwave spectroscopy and the application of Stark deceleration methods to guide, decelerate and focus Rydberg Ps beams. In this talk I will discuss recent examples of such experiments and what may be possible in the near future.

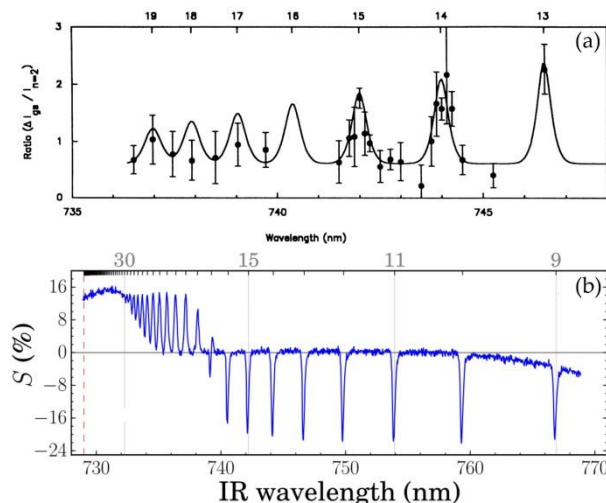


Figure 1 Spectra of Rydberg Ps excitation conducted in (a) 1990 [4] and (b) 2015 [5]. The difference in data quality is entirely due to different detection methods.

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Techniques for production and detection of a 2^3S positronium beam

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In this work, we show recent measurements of 2^3S long-lived positronium production via spontaneous decay from 3^3P level [1, 2]. The possibility to tune the velocity of the 2^3S positronium, excited following this scheme, is also presented [2].

In the light of these results, we discuss the use of the $3^3\text{P}\rightarrow 2^3\text{S}$ transition to realize a monochromatic pulsed 2^3S positronium beam with low angular divergence in view of future possible deflectometry/interferometry experiments. The apparatus developed for this aim is described and preliminary tests of 2^3S beam production are presented. The possibility to overcome the natural $3^3\text{P}\rightarrow 2^3\text{S}$ branching ratio via stimulated emission, and thus increasing the intensity of the 2^3S source, is also demonstrated [3]. A position-sensitive detector for a pulsed beam of slow positronium, with spatial resolution lower than $100\ \mu\text{m}$ [4], is finally described in view of its possible application for the spatial characterization of the 2^3S beam.

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A Multi-ring Electrostatic Guide for Rydberg Positronium

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If positronium (Ps) atoms are excited to Rydberg-Stark states their lifetimes can be significantly increased [1], and they may possess large electric dipole moments [2]. These properties can be exploited to produce a long-lived Ps beam using inhomogeneous electric fields, which has been previously demonstrated in a continuous quadrupole device [3]. Here we present measurements made using an electrostatic guide comprising a multi-ring electrode structure. This configuration allows time-varying potentials to be applied to individual electrodes, and can in principle decelerate and trap Ps atoms [2]. Our measurements are in good agreement with particle trajectory calculations and show that Ps atoms may be guided and focused in this device, which can also facilitate crossed beam scattering experiments [4]. Applications to future deceleration and trapping will be discussed.

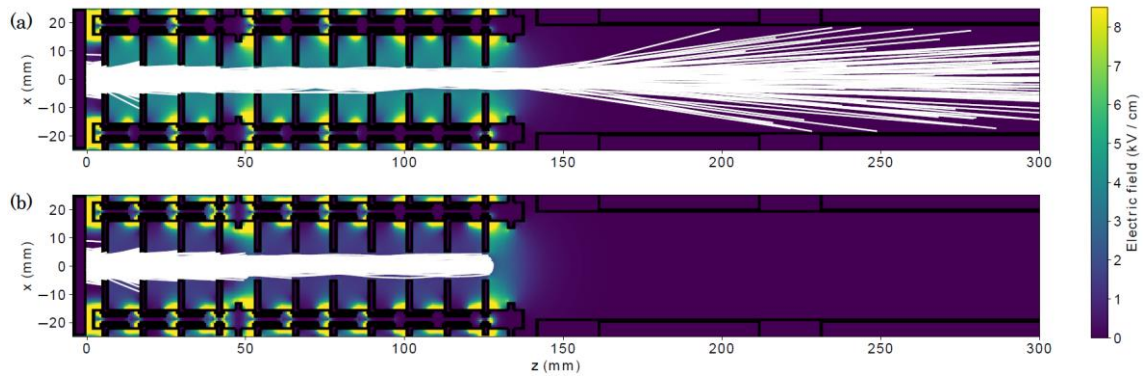


Figure 1 Calculated trajectories of (a) $n = 13$ and (b) $n=19$ Ps atoms guided through a multi-ring electrode structure. The $n=19$ atoms ionize at the large potential between the final electrode and the grounded flange whereas the $n=13$ atoms propagate into the flange. Different potentials were applied to each case to demonstrate field ionisation.

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Precision microwave spectroscopy of the $n=2$ positronium fine structure.

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As a purely leptonic system, positronium (Ps) is an ideal system for performing QED tests [1]. QED corrections to Ps energy levels have been calculated up to order $m\alpha^6$, and the theoretical calculations [2] are currently more precise than experimental measurements. The first measurement of the $n = 2$ fine structure was of the $2^3S_1 - 2^3P_2$ transition, conducted in 1975 by Mills, Berko and Canter [3]. This measurement was improved upon by Hatamian, Conti and Rich, in 1987 [4], and then by Hagen and co-workers in 1993 [5]. However, these experiments all relied on generation of Ps atoms in the 2^3S_1 state via positron bombardment into metal targets [6], which is intrinsically inefficient and necessarily results in Ps with energies of several eV. The last fine structure precision measurements are now over 25 years old, with uncertainties of approximately 200 ppm [5]. Here we present the results of a new Ps $n = 2$ fine structure measurement ($2^3S_1-2^3P_2$) in which 2^3S_1 atoms were produced via laser excitation [7]. This methodology is more efficient and results in the production of much slower atoms, significantly reducing systematic errors.

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Recent progress towards positronium Bose-Einstein condensation

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Ortho-Positronium (o-Ps) is one of the best candidates for the first Bose-Einstein condensation (BEC) of any system which contains antimatter. Ps-BEC can be used to measure antimatter gravity using an atomic interferometer. It can also be used as a source for a 511-keV gamma-ray laser. We proposed a new scheme to realize Ps-BEC using a positron focusing system and fast cooling of Ps [1]. Our target density and temperature for Ps-BEC is $\sim 10^{17}$ cm⁻³ at ~ 10 K. A schematic view of the proposed setup is shown in Fig. 1. We are currently trying laser cooling of Ps at KEK slow positron facility (SPF). Recent experimental progress in the following components of the Ps-BEC setup will be discussed: the positron focusing system using multi-stage brightness enhancement system, Ps generator/condenser/cooler target material, and special home-made 243 nm pulsed laser system for Ps laser cooling.

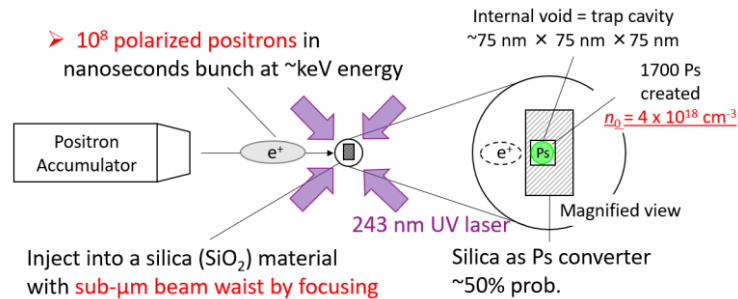


Figure 1 Conceptual view of the experimental setup. Focused positron bunches from a positron accumulator are injected into a cold silica cavity in which Ps cloud of 4×10^{18} cm⁻³ are created. Ps are then cooled by thermalization and 243 nm laser cooling.

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Studies of quantum entanglement in positronium decay with the J-PET detector

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J-PET is the positron-emission tomograph (PET) constructed from plastic scintillators. It is optimized for the detection of photons from electron-positron annihilation [1,2,3,4]. Such photons, having an energy of 511 keV, interact with electrons in plastic scintillators predominantly via the Compton effect. According to Klein-Nishina formula polarization of a photon might be estimated by measurement of the momentum direction of primary and scattered photon. By investigating correlations between polarization vectors we are able to determine the initial state [5,6]. Predicted by theory but never experimentally proven, the two- and three-photon states should be entangled. In this talk I will present a method to determine single photons polarisation, correlations between polarisations as well as quantum information theoretic version of the Klein-Nishina formula in order to determine whether initial state was separable or entangled.

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Search for \mathcal{T} -violation in Positronium decay using the J-PET detector

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Time reversal symmetry (\mathcal{T}) violation has been one of the most intriguing aspects of the tests on discrete symmetries. So far, \mathcal{T} -violation has not been observed in purely leptonic systems [1, 2, 3]. According to the standard model predictions, photon-photon interaction or weak interaction can mimic the symmetry violation at the level of 10^{-9} (photon-photon interaction) and 10^{-13} (weak interactions) respectively, posing as a physical restriction to these tests [4-6].

The Jagiellonian Positron Emission Tomograph (J-PET) developed at Jagiellonian University in Krakow, Poland, is one of its kind being based on organic scintillators [7, 8, 14]. J-PET is an axially symmetric and high acceptance scanner that can be used as a multi-purpose detector system. It is well suited to pursue tests of discrete symmetries in decays of positronium in addition to medical imaging [9, 10, 12, 14]. J-PET enables the measurement of the momentum vector \mathbf{k}_i and the polarization vector $\mathbf{\epsilon}_j$ of annihilation photons [10, 11, 13]. Measurement of polarization of annihilation photons is a unique feature of the J-PET detector which allows the study of \mathcal{T} -violation by determining the expectation values of the time reversal symmetry odd operator [10],

$$(\mathbf{\epsilon}_j \cdot \mathbf{k}_i), \text{ (for } j \neq i) \quad [10].$$

J-PET collaboration aims to improve the sensitivity for the tests of the time reversal symmetry with respect to the previous experiments in the leptonic sector beyond the present established level of 10^{-3} [2]. At the turn of 2017 and 2018, a three month data-taking campaign with the positronium produced in the porous polymer was conducted. The results of the analyzed data will be presented in the conference.

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Studies of ortho-positronium decays into three photons with the J-PET detector

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The Jagiellonian Positron Emission Tomograph (J-PET) setup, besides being the first PET scanner built with plastic scintillators [1,2] is currently used to conduct a broad range of experiments involving ortho-positronium (o-Ps) decays into three photons [3,4].

We will present results of studies of o-Ps $\rightarrow 3\gamma$ decays performed in J-PET with a view to searching for angular correlations between the photons' momenta and positronium spin direction which would violate the combined CPT symmetry, scarcely tested in leptonic systems. To date, the most precise CPT test using ortho-positronium decays reached the precision of 3×10^{-3} [5] whereas effects limiting the sensitivity are only expected at the level of 10^{-9} [6].

In the discussed J-PET measurement, ortho-positronium atoms are created by positrons from a ^{22}Na source thermalizing in an extensive-size cylindrical target of porous XAD4 material and decay positions are reconstructed using a trilateration-based technique [7]. Decay photons are recorded by 192 strips of plastic scintillators with high timing resolution. Such a setup (presented in Figure 1) allows for registration of an unprecedented spectrum of geometrical configurations of o-Ps $\rightarrow 3\gamma$ decays including also correlations with positronium spin.

Angular and energetic relative distributions of the decay photons will be presented along with the current stage of studies of a CPT-odd angular correlation operator $\hat{S} \cdot (\hat{k}_1 \times \hat{k}_2)$ where \hat{S} denotes positronium spin direction and \vec{k}_i are momentum vectors of the annihilation photons ordered so that $|\vec{k}_1| > |\vec{k}_2| > |\vec{k}_3|$. With an angular resolution and o-Ps polarization control improved with respect to previous measurements, J-PET aims at achieving the sensitivity of such CPT test at a precision level of at least 10^{-4} .

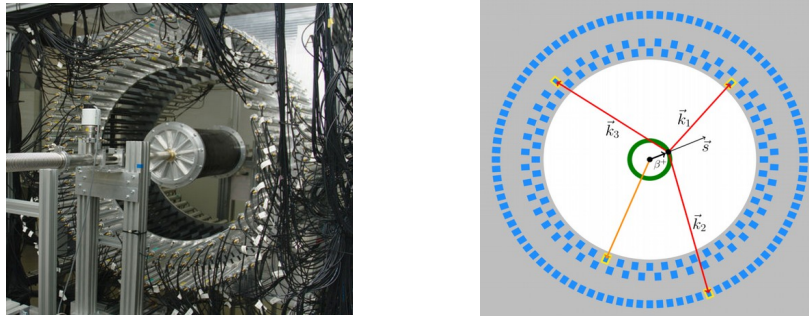


Figure 1 A cylindrical target ($r=12$ cm) for o-Ps formation inside the J-PET detector (left) is used to estimate the ortho-positronium spin in every event using positron polarization (right).

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Charge symmetry test in decays of positronium atoms using the J-PET detector

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Discrete symmetries (reflection in space (P), reversal in time (T) and charge conjugation (C)) are violated in weak interactions only. Charge conjugation transforms a particle into antiparticle and vice versa by changing its internal quantum numbers. Thus, the Charge symmetry studies can contribute to resolve the ambiguity in excess of matter over antimatter in the Universe. Positronium atom (Ps) which is the meta-stable bound system of particle (e^-) and its antiparticle (e^+) can be an excellent tool for studying the charge symmetry violation [1-3]. In 1967, Mills and Berko measured the C-forbidden decays of the singlet state (1S_0 : p-Ps) by estimating the ratio (R) of its decays $3\gamma / 2\gamma$ with best limit so far ($R \sim 2.6 \times 10^{-6}$ at 68% confidence level) [4].

J-PET is the PET device built from 192 plastic scintillators of dimension $500 \times 19 \times 7 \text{ mm}^3$ which are arranged axially in 3-layers [5-8]. It is used to investigate the C-forbidden decays of the positronium atoms ($p\text{-Ps} \rightarrow 3\gamma$) and estimate the branching ratio between 3γ to 2γ [2]. The event wise registration of the annihilation photons emitting from the decay of positronium atoms allow to distinguish either they are originating from the long-lived (o-Ps in range of ns) or short-lived (p-Ps in range of ps) atoms [9-10]. Furthermore, the angular correlation between the emitting photons can also be used as a signature to differentiate between the decays either from singlet (p-Ps) or triplet (o-Ps) states of the Ps atom. Moreover, the plastic scintillators used in J-PET offers the excellent time and high angular resolution and thus the value of R is expected to be measured with better sensitivity [5,6]. First results from the studies in the framework of J-PET detector will be presented and discussed.

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TOT method for the disentanglement of photons in Positron Annihilation Lifetime Spectroscopy

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The Jagiellonian Positron Emission Tomograph (J-PET) is the first PET built from plastic scintillators [1-5]. It is designed to studying the properties of positronium atoms and their implications for the medical imaging as well as in discrete symmetries tests [6-8]. In order to take advantages of the fast signals and low pileups in plastic scintillators the Time-Over-Threshold (TOT) method is adopted instead of measurement of charge as a response to energy deposition. The application of TOT method enables the fast signal processing reducing significantly signal acquisition dead time in comparison to crystal scintillator and providing the compactness of signals readouts. The signals are recorded using a Multi-Voltage Threshold mezzanine (MVT) board to probe signals at four fixed thresholds in voltage domain (within the accuracy of 20 ps RMS) which are based on Field Programmable Gate Arrays (FPGA) [9-10] .

In plastics, the photon interacts via Compton scattering depositing part of its energy and impede in identifying the exact energy of the interacting photons originating from the direct annihilation ($e^+e^- \rightarrow 2\gamma$) or from various possible decays channels of Positronium atoms (para-Positronium, ortho-Positronium, pick-off process). To use the potential of the TOT technique, an algorithm was developed for tagging the photons of different energies. Furthermore, a detailed analysis was performed to establish the relationship between TOT and energy deposition in a single interaction of photons based on the scattering angle via registration of primary and scattered photon positions. Results from the analysis will be presented and discussed.

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Open volumes structure and molecular transport in polymer and biopolymer nanocomposites

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We will discuss gas transport mechanisms in polymer nanocomposite in which fillers of different nature and concentration are added [1-5]. The kinetics of gas transport was studied by gas phase permeation techniques and free volumes were analyzed by positron annihilation lifetime techniques (PALS) with a fast-fast lifetime apparatus and with PLEPS beam at NEPOMUC facility. Gas barrier properties of two biopolymer nanocomposite films will be discussed in relation of their fractional free volume. The first biopolymer film is poly(3-hydroxybutyrate-co-3-hydroxyhexanoate) (PHBH) containing 0.25 wt. % of Graphene Oxide (GO) filler nanoparticles: PHBH is a biodegradable polymer that can be obtained either by microorganisms or chemical synthesis. The second biopolymer film is poly(lactic acid) (PLA) in which cellulose nano-fibrils have been dispersed with content ranging from 0 to 15 weight %. It will be shown that in both biopolymer films the filler addition improves their gas barrier properties but with different mechanism. Introduction of GO in PHBH induces an increase of the gas impermeable PHBH crystalline fraction while introduction of cellulose nanofibrils in PLA modifies the structure of the PLA layers at the matrix-filler interface.

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Long-lived Positronium for pulsed antihydrogen production

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The foreseen production of cold antihydrogen atoms at CERN's Antiproton Decelerator (AD) opened up the possibility to perform direct measurements of Earth's gravitational acceleration on antimatter bodies [1]. This is the primary goal of the AEGIS collaboration: measure the value of g using a moiré deflectometer/Talbot-Lau interferometer with a pulsed source of cold, neutral atomic antimatter [2].

This talk is focused on the milestones achieved by AEGIS along the first development of a pulsed source of cold antihydrogen using charge-exchange between trapped antiprotons and cold Rydberg positronium [3]. Cold antiproton plasmas were first prepared with well-established techniques in a custom Malmberg-Penning trap with partially open electrodes to allow Rydberg Ps atoms to enter the trap [4] [5]. Ps was subsequently formed and detected in the cryogenic, high magnetic field environment of the experiment using Single-Shot Positron Annihilation Lifetime Spectroscopy (SSPALS) [6]. The crucial ability to manipulate it optically via pulsed laser beams was achieved thanks to a newly developed detection method based on a cryogenic Micro-Channel Plate (MCP), able to spatially image photo-positrons from Ps photo-dissociation events with a resolution of ~ 100 μm [7]. Thanks to this high-resolution imaging detector, the accurate measurement of the Ps atoms' velocity distribution emitted from the cryogenic target and the optimization of the charge-exchange cross-section with antiprotons were possible. Furthermore, this detector provided shot-by-shot diagnostics of Ps Rydberg excitation and alignment towards the antiprotons in the trap for the first experimental trials of pulsed antihydrogen production.

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ortho-Positronium annihilation in Room Temperature Ionic Liquids

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Melting temperatures of Room Temperature Ionic Liquids (RTILs) are lower than 100°C. They have very unique properties, and they show many interesting phenomena. There are many new application for many different fields. One of them is the spent nuclear fuel reprocessing. Therefore the irradiation effects such as the research of excess electrons, for example the mechanism of solvation, is very important. Electron solvation is usually very fast process. According to the spur reaction model [1], positronium (Ps) formation in insulation materials are caused by the very fast, ~ps, reaction of a thermalized positron and one of excess electrons. Therefore, the positron annihilation method can be a strong tool to investigate fast reactions of excess electrons. It was initially the reason of the positron annihilation experiments for RTILs. Recently, it was reported that the Ps bubble in RTILs showed some phenomena that were very different from them observed in other molecular liquids. [2,3] Now the reason of these interesting phenomena is being understood. The structure caused by the ionic interaction between anions and cations can exist even at the higher temperatures than the melting temperatures. It was the reason why the oscillation of Ps bubble was observed at the temperatures near the melting temperatures in RTILs. The small temperature dependence of the Ps bubble size is also, probably, caused by this ionic structure. Therefore, we decided to investigate the temperature dependence of the Ps bubble size in wider temperature range, i.e. higher temperatures. The vertical positron beams installed at AIST is suitable apparatus to investigate RTILs, because it is possible to inject positrons from the side of liquid surface. We are discussing the results of the positron annihilation lifetime measurements performed by the AIST positron beam for RTILs.

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INTI plot - a new standard for the presentation of PALS results

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The Ps is accepted as a convenient probe of structure – the lifetime of ortho-Ps substate depends on the size of free volume (void) where the o-Ps is trapped, while the o-Ps intensity is correlated with the concentration of free volumes. These two parameters, τ_{o-Ps} and I_{o-Ps} are usually considered to be reliable quantities informing about the reaction of the system to influence of external factors. It was assumed to conclude about structural changes based on changes in (τ_{o-Ps} , I_{o-Ps}) parameters occurring in the function of external factors (temperature, pressure) and present results as a function of these factors. As we have shown on the example of selected *n*-alkanes [1], on the INTI plot (the INTensity, lifeTime plot, the results in the form of a curve in the (τ_{o-Ps} , I_{o-Ps}) coordinates), we can draw new conclusions, including those independent of the length of the hydrocarbon chain, common for the whole group of compounds. Analyzes of experimental data for other compounds (including derivatives of alkanes, selected polymers) have shown that, similarly to alkanes, the presentation of results on the INTI plot allows us to look at the results from a different perspective and draw additional conclusions. The results obtained in the form of INTI plot for selected polymers and organic compounds will be presented.

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Ps formation and dissolved oxygen in liquids

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Recently, the phenomenon of shortening of the ortho-positronium lifetime (quenching) in various liquids due to its interaction with dissolved oxygen (O₂) drew notable attention. This effect is significant when applying positron annihilation spectroscopy to study healthy and cancerous tissues of living organisms, due to the fact that the O₂ content in these tissues is remarkably different [1]. These studies are also stimulated by the development of a new type of positron annihilation tomograph aimed on detection of oncological diseases, which is constructed at the Jagiellonian University in Krakow [2].

Here we present the results of PALS experiments in organic liquids (cyclohexane, isooctane, isopropanol) and water. Our aim was to determine the rate constants of interaction of the dissolved oxygen with the Ps atom. These experiments are also the first step towards studies of unusual properties of water pool in inverted micelles in organic solvents.

In our previous experiments we used the freeze-thaw method in order to remove the dissolved O₂ from liquids, but we stopped doing this because the positron source immersed in a frozen liquid could be damaged. Instead we developed a setup that removes oxygen from liquid phase by means of bubbling the argon gas through it. All gases used in experiments were cleaned from impurities (passing through alkali and 3 Å nanosieve). All studied liquids were also perflated with air and pure oxygen, to provide more accurate determination of the Ps + O₂ reaction rate constants.

A computer software has been developed for fitting the LT spectra, which uses values with clear physical meaning (rate constants of chemical reactions with participation of Ps, annihilation rates of different positron states, probability of the Ps formation in a quasifree state, typical formation time of a Ps nanobubble) as adjustable parameters. Processing of the spectra allowed to identify dominant interaction of the Ps atom with dissolved oxygen. It comes out to be mainly ortho-para-conversion (ortho-Ps ↔ para-Ps), but not the oxidation (Ps + O₂ → e⁺ + O₂⁻). Values of the reaction rate constants are obtained.

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New Physics with Positron Traps and Trap-Based Beams

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The development of novel positron traps and beams has enabled new investigations of anti-matter. This talk will discuss highlights of recent successes and the critical tools that enabled them. It will conclude with a brief discussion of prospects for further technological progress and the new physics that it might enable.

Studies of antimatter are of interest for a range of scientific and technological applications, including fundamental tests of gravity and tests of symmetries predicted by field theories (e.g., CPT), understanding astrophysical processes, and the characterization of materials. Many applications benefit greatly from tailoring collections of the antiparticles to optimize them for a specific use. Unlike electrons, which are copious in our world of matter, positrons are scarce (e.g., currents of picoamps instead of amps). The need to keep positrons isolated from ordinary matter has motivated the development of methods to manipulate them in vacuum in the form of single-component gases and plasmas.

More than three decades of positron trap and beam development have enabled specially designed electromagnetic traps for long-term (e.g., weeks or more) antimatter confinement, cryogenically cooled antiparticle gases and plasmas, high-density plasmas, finely focused beams, and methods to deliver very large bursts and/or short temporal bursts of antiparticles and to create guided positronium (Ps) atom beams [1, 2].

Scientific and technological progress in several areas will be reviewed. It includes the creation and study of antihydrogen atoms and gravity tests [3, 4, 5, 6]; the formation of the positronium molecule (i.e., Ps_2 , the first many-electron, many-positron state, $e^+e^-e^+e^-$) [7]; and understanding Feshbach-resonances in positron annihilation and the nature of the resulting positron-molecule bound states [8]. Outstanding goals and the challenges associated with them will be discussed. They include the opportunities that could be enabled by putting a positron trap system on an intense source such as the NEPOMUC facility in Munich, and plans to study the electron-positron system [9], namely a positronium-atom Bose-Einstein condensed gas (BEC) [10] and a classical "pair" (i.e., $e^+ - e^-$) plasma [11].

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Annealing behaviours of open spaces in thin Al₂O₃ films deposited on semiconductors studied using monoenergetic positron beams

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Metal-oxide-semiconductor gate stacks for GaN-based power devices have been studied extensively. The deposition of gate oxides is known to introduce carrier traps at the interface, and they are the major obstacles in device fabrication. Because the interfacial reaction of the insulator and GaN could occur easily, knowledge on the interface reaction between oxides and GaN is a key to developing GaN-based MOS devices. We used monoenergetic positron beams to study reactions between Al₂O₃ and GaN and annealing behaviors of open spaces in Al₂O₃ [1]. 25-nm-thick Al₂O₃ films were deposited on GaN by using ALD method. After the deposition, the samples were annealed up to 900°C for 5 min in N₂ atmosphere. Figure 1 shows *S*–*E* curves for Al₂O₃/GaN before and after annealing treatments. The *S* value at *E*≅1 keV corresponds to the annihilation of positrons in the Al₂O₃ film. After annealing at 800°C, observed increase in *S* at *E*=2 keV was due to the trapping of positrons by vacancies introduced by the reaction between Al₂O₃ and GaN. The inset shows the depth distributions of *S* obtained from fitting. The lifetime spectra of positrons in Al₂O₃ were measured, and they were decomposed into three components. For as-deposited sample, the values of τ_1 , τ_2 , and τ_3 were obtained as 0.262 ns (54%), 0.580 ns (45%), and 1.77 ns (1%) respectively. The positron lifetimes in γ -Al₂O₃ were simulated. Fig. 2 shows the atomic configurations used in the calculation and positron density distributions.

It was found that τ_1 agreed with the calculated positron lifetimes for clusters of V_{Al} . Annealing behaviours of open spaces in Al₂O₃ was discussed based on the experiments and simulation.

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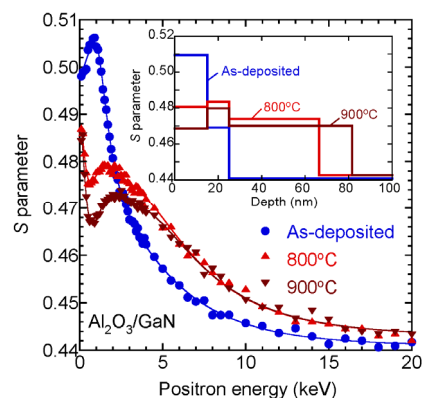


Fig. 1 *S*–*E* curves for Al₂O₃/GaN. The inset shows the depth distributions of *S*.

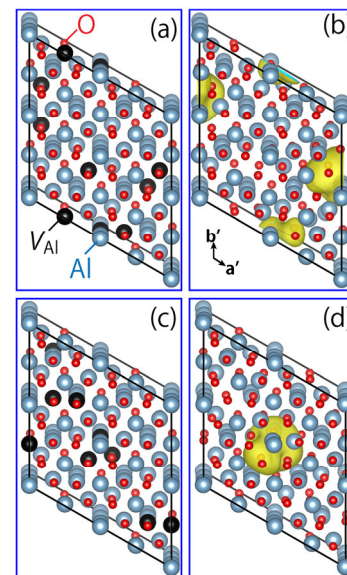


Fig. 2 Atomic configurations of γ -Al₂O₃ [(a) and (c)] and distributions of positron densities [(b) and (d)].

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A novel high-brightness and energy-tunable positronium beam and future applications

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The first, high-brightness and energy-tunable positronium (Ps) beamline produced using the photodetachment of positronium negative ions (Ps⁻) has been recently constructed at Tokyo University of Science [1]. Slow positrons are generated by a ²²Na source (740 MBq) in conjunction with a solid Ne moderator. The positrons are accumulated in a buffer-gas trap to form a ns-pulsed (50 Hz) positron beam that is synchronized with the pulsed laser beam for the Ps⁻ photodetachment. The positron beam extracted from the trap is electrostatically accelerated and focused onto a W (100) film of 100-nm thickness using a magnetic lens. Ps⁻ ions are efficiently emitted in a transmission geometry from the downstream surface of the W thin film that is coated with a sub-monoatomic Na layer. The Ps⁻ ions are electrostatically accelerated to the desired kinetic energy and photodetached by a Nd:YAG IR laser beam (0.2 J cm⁻², 1064 nm). This way an energy-variable Ps beam in the kinetic range 0.2-3.3 keV is obtained. The Ps atoms are detected by a position sensitive detector located 419 mm downstream of the photodetachment point in a differentially-pumped chamber.

The successful performance of the beamline has already been thoroughly characterized [1]. Several kinds of experiments are currently being carried out and planned using this beamline. These include the detection of the hyperfine transition between ortho- and para-Ps when passing through a multi-layered transmission magnetic grating [2], measurements of Ps scattering from crystal surfaces in a grazing-angle geometry [3] and the observation of the interference of Ps wave functions transmitted through a single layer of graphene.

Absolute cross sections measurements of the inner-shell ionization of the atomic K- and L-shells of thin film targets, such as Cu and Ag, by Ps impact are also planned. The knowledge of those cross sections will allow us to clarify the role of the fundamental interactions in the scattering process involving a composite antimatter-matter system, as cross sections by electron and positron impact are quite different [4]. Those measurements are also important for a better understanding of the dynamics of the inner-shell ionization process for the development of accurate scattering theories.

The details on the plan and progress of these experiments will be presented at the conference.

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Positron binding, scattering, and annihilation on atoms and molecules

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The ability of the positron to bind to molecules is key to the strong enhancements of positron annihilation rates in polyatomic molecules [1]. This enhancement is due to positron capture in vibrational Feshbach resonances, observation of which has led to measured values of positron binding energies for over 70 molecules [2]. *Ab initio* calculations of positron binding to nonpolar molecules have proven to be extremely challenging. Here, we use a model-potential approach [3] to calculate elastic *s*-wave scattering cross sections, annihilation rates, and (where applicable) binding energies for positron interactions with atoms and small nonpolar molecules, namely, Be, Mg, He, Ar, H₂, N₂, Cl₂, and CH₄. We write the positron-molecule interaction potential as $V(\mathbf{r}) = V_{\text{st}}(\mathbf{r}) + V_{\text{cor}}(\mathbf{r})$, where $V_{\text{st}}(\mathbf{r})$ is the electrostatic potential of the target, and $V_{\text{cor}}(\mathbf{r}) = -\sum_A (\alpha_A/2|\mathbf{r} - \mathbf{r}_A|^4) \{1 - \exp[-(|\mathbf{r} - \mathbf{r}_A|/\rho_A)^6]\}$ is a model correlation potential, where the sum is over the target's constituent atoms A , with the nucleus at position \mathbf{r}_A and the hybrid polarizability α_A [4]. The cutoff parameters ρ_A are taken from Ref. [5] for Be, Mg, and He; for Ar we choose it to reproduce the accurate *s*-wave scattering phase shift from many-body-theory calculation [6]; for C and N we use the same value as for H, while for Cl we use the same value as for Ar (due to the similar radii of these atoms). Scattering data are obtained by correctly normalizing Gaussian-based positive-energy positron eigenstates. Our calculations confirm positron binding for Be and Mg, and predict it for Cl₂. Figure 1 shows the annihilation parameter Z_{eff} as a function of positron momentum for all of the species, along with existing calculations. The very large values of Z_{eff} at small momenta for Cl₂, Be and CH₄ are due to the presence of a weakly bound state or low-lying virtual level. The discrepancy with the result of Ref. [5] for Mg is due to the presence of a *p*-wave shape resonance not accounted for here.

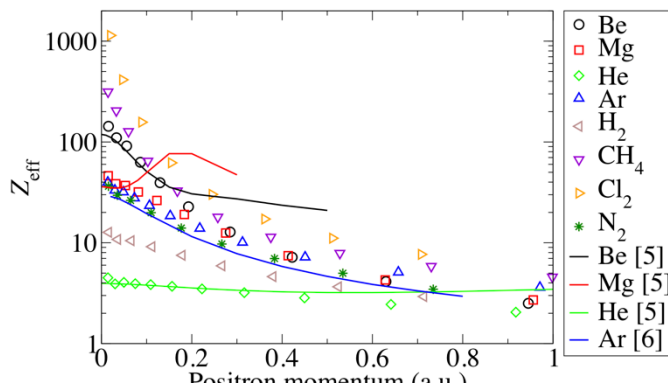


Figure 1 Annihilation parameter Z_{eff} for Be, Mg, He, Ar, H₂, N₂, Cl₂, and CH₄. Symbols: present results. Lines: previous calculations.

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Simulating positron to positronium conversion in nanostructured materials

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Silicon-based nanochanneled converters (NCPs) for the production of cold Positronium (Ps) have been introduced in 2010 [1,2,3] and since then provided a reliable source of cold Ps to a variety of experiments [4,5,6,7,8].

With the goal of advancing the optimization of such converters we have formulated a classical model to describe the production and cooling of Ps in NCPs [9,10]. The simulation of such process poses several challenges due to the complexity of the geometry in which it takes place. We will here briefly present our model and discuss several simplifications of the simulation process which, without altering significantly the simulation results, reduce the computational costs enough to allow for systematic scans of the NCP construction parameter space.

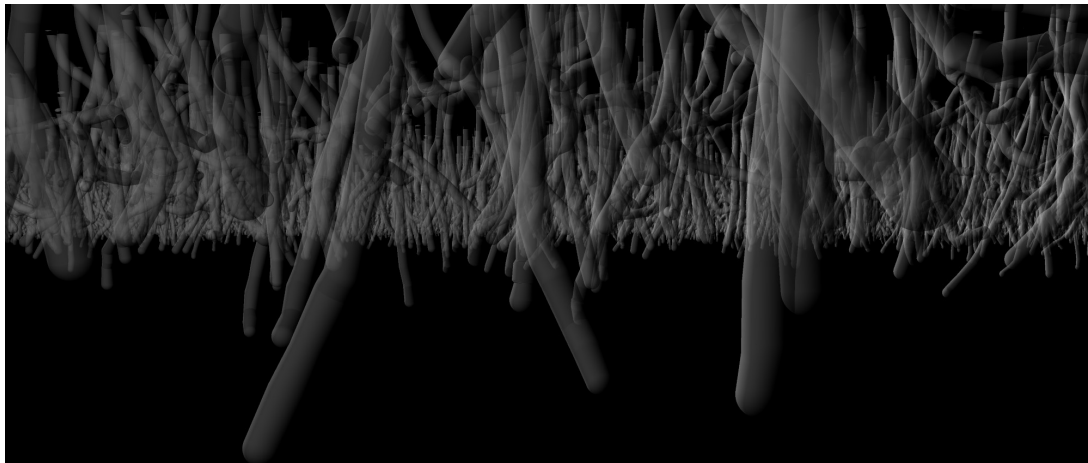


Figure 1 3D rendering of a geometric model of the nanoscopic channels in an NCP converter

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Accumulation of positrons from a linac based source

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The aim of the GBAR experiment is to measure the effect of gravity on antihydrogen atoms [1]. Those are created by interactions of antiprotons with a dense positronium cloud. The antiprotons are obtained from the decelerator complex at CERN now composed of two steps: the Antiproton Decelerator, in which the beam reaches 5 MeV energy, and ELENA where it is further decelerated to 100 keV. Positronium (Ps) is obtained by implantation of 4 keV positrons onto a mesoporous silica film. The goal is to obtain a cloud of the order of 10^{10} positrons. In order to obtain the necessary intense positron beam, a 9 MeV linac, accelerates electrons toward a tungsten target equipped with a mesh moderator. The resulting slow positron beam is then transported to a buffer gas trap where particles are cooled by interaction with nitrogen and CO₂ and accumulated in a 5T multi-ring Penning-Malmberg trap.

We present the performances of trapping and accumulation of positrons.

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The new positron beam line of the GBAR experiment at CERN

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The aim of the GBAR experiment is to measure the gravitational acceleration of antihydrogen, the simplest anti-atom formed by an antiproton and a positron. Direct measurement of the acceleration requires anti-atoms at extremely low temperature, well below the limit of cooling neutral particles. The distinctive idea behind GBAR is to cool positively charged antihydrogen ions with the help of laser-cooled ordinary matter atoms in several steps to the 10 microkelvin range. The cold anti-ion is then neutralized by photodetachment of a positron and the time until annihilation on the wall of the experimental chamber is measured to determine the acceleration. Antihydrogen ions are created in two consecutive reactions in a dense positronium cloud. Positrons are generated by a 9 MeV linear energy accelerator (linac), slowed down and shortly stored in a buffer gas trap and accumulated in a 5T multi-ring Penning-Malmberg trap. The accumulated particles are ejected from the trap, accelerated to 4 keV and implanted into a positron-positronium conversion target, placed in a magnetic field free target chamber. The conversion target is a thin mesoporous silica film, deposited on silica single crystal. The new ELENA facility at CERN supplies antiprotons at 100 keV kinetic energy for the experiment. GBAR will add later a Penning-Malmberg trap to optimize the antiproton pulses. A proton source is installed to test the beamline and measure the cross section of the matter equivalent of the relevant reactions.

The experimental setup has been installed in the AD Hall at CERN. The linac, the positron beamline and the two positron traps are operational and we demonstrated efficient positronium creation in the conversion target. The experimental setup has been shortly tested with antiproton pulses from the ELENA antiproton decelerator ring. During LS2 (Long Shutdown 2, until 2021) we will improve the positron line, install the antiproton trap and measure reaction cross sections using the GBAR proton source.

We present the experimental setup and discuss the performance of the positron beamline.

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Antimatter wave interferometry. First observation

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Interference of matter waves is at the heart of quantum physics and has been observed for a wide range of particles from electrons [1,2] to complex molecules [3]. In this work will be demonstrated matter wave interference of single positrons using a period-magnifying Talbot-Lau interferometer [4]. The system produced high contrast periodic fringes (see an example in Fig. 1), which were detected by means of nuclear emulsions capable of determining the impact point of each individual positron with submicrometric resolution. The measured energy dependence of fringe contrast in the range of 8 to 16 keV proves the quantum-mechanical origin of the periodic pattern and excludes classical projective effects, providing the first observation to date of antimatter wave interference. Some of the future applications of this interferometric technique will be illustrated, including decoherence studies and measurement of the gravitational acceleration of neutral antimatter systems that take advantage of the inertial detection capabilities of Talbot-Lau interferometry.

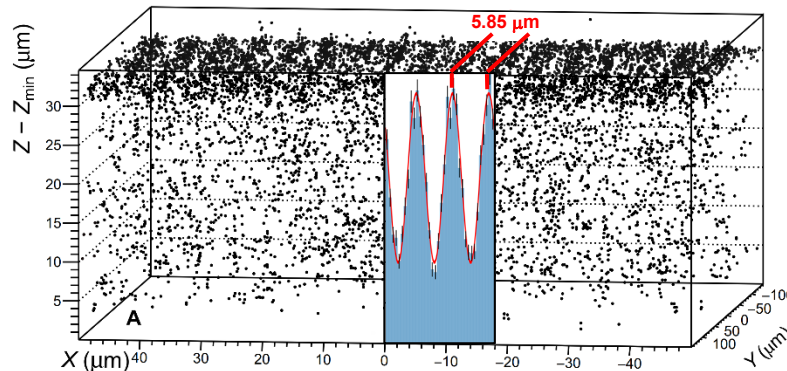


Figure 1 Three-dimensional distribution of the reconstructed clusters limited to a 100-mm-wide region along X. A hint of the periodic fringes is even appreciable by visual inspection. The inset shows a histogram of the experimental points and a sinusoidal fit for the highest contrast view (error bars represent poissonian counting uncertainties).

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Development of a PbWO₄ detector for single-shot positron annihilation lifetime spectroscopy at the GBAR experiment

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The GBAR experiment plans to produce anti-hydrogen atom and ion by anti-proton beam collision with ortho-positronium (o-Ps) [1]. A slow positron beam line producing short intense positron pulse has been developed to produce an o-Ps cloud with high density (up to 10^{12} o-Ps/cm³) inside a cavity shaped target which is required to produce anti-hydrogen ions. To measure the cross-section of anti-hydrogen atom and ion, precise measurement of o-Ps density is important in order to reduce systematic uncertainty.

A fast detector composed of PbWO₄ crystal and a photomultiplier tube (PMT) has been developed to measure the intensity of positron beam and density of the o-Ps cloud. This type of detector assembly has proved having good time resolution in a previous study [2]. With a few photo-electron detection per 511keV γ -ray, not only large dynamic range can be achieved but also calibration of a single γ -ray signal is feasible to measure absolute efficiency. A Na-22 radioactive source has been used for energy calibration, for measurement of the detection efficiency and time response.

To achieve precise measurement, a method to take account of Compton background has been developed to reduce a bias in positron beam intensity and o-Ps density. To reduce a systematic uncertainty from mobility of o-Ps with angular spread, a simulation based on Geant4 package [3, 4] has been developed. A method to measure the angular spread has been developed based on simulation.

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The Generation of Ultra-relativistic Positron by Gas-Solid Target Based on Ultra-intense Laser

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Recently the ultra-relativistic positron beam was produced via the interaction between ultra-intense laser and gas-solid targets[1-2]. In the experiments, the positrons and the electrons were separated by magnetic field after passing through the collimator, and the energy spectras of positrons and electrons were given by the Image Plates (IPs). The results showed that the positron beam above 1MeV temperature was produced and the average positron yield was $\sim 5.33 \sim 5.33 \times 10^7$ /shot. In addition, a model of solving the wakefield electrons energy spectrum was established based on the maximum entropy method (MEM). Meanwhile, the simulation results by Monte Carlo agreed well with the experimental results.

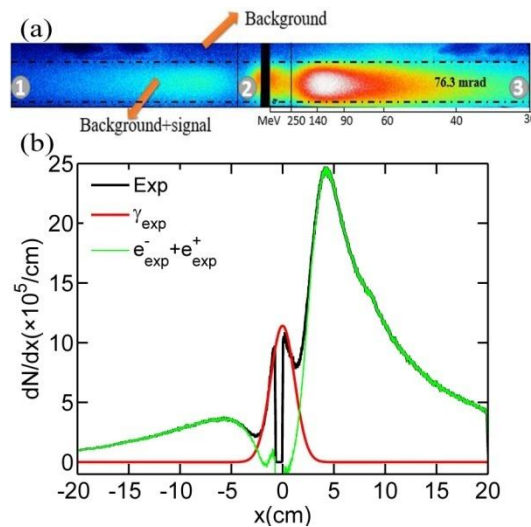


Figure 1 (a) Typical signal of positrons and electrons recorded on IPs of 5 shots; (b) The black line is the integrated signal of IPs. The red line is the gaussian fitted photon signal. The green line is the real signal of electrons and positrons.

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Generation of quasi-monoenergetic high energy positrons based on laser wakefield accelerated electrons

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Great progress has been made on laser wakefield accelerators (LWFA) [1], more than 8 GeV electron beam from LWFA has been reported recently. Such energetic electron beam from LWFA is proposed to produce energetic positrons recently. A new scheme for generating energetic positron beam by irradiating LWFA (Laser wakefield Accelerator) electrons on solid targets is studied both theoretically and experimentally. In our simulations, the process is studied by PIC code PLASIM [2] and Monte-Carlo Code Fluka. Based on our simulations, corresponding experiments has been designed and conducted on the 200 TW laser facility in Shanghai Jiaotong University. For the first time in China to the best of our knowledge, energetic positrons produced by LWFA electrons have been observed in our experiments [3]. Simulation results are in good agreement with the experimental ones.

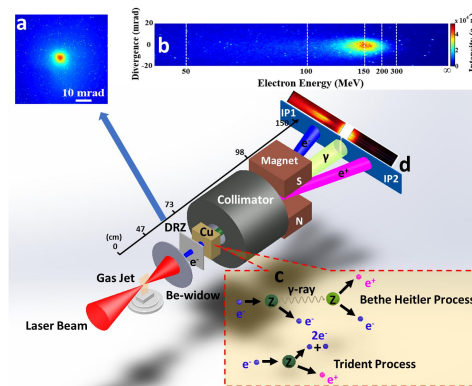


Figure 1 Experimental setup for generation and detection of positron beams based on laser-plasma accelerated electron beams impinging on a Cu target. (a) Typical profile of the laser wakefield-accelerated electron beams. (b) Typical measured spectrum of electron beam without the Cu target. (c) Two physical mechanisms for positron generation. (d) Raw signal of positron and secondary electron, as recorded by the two IPs, by accumulating 120 laser shots

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Positron-Induced Luminescence

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Cathodoluminescent materials, in addition to being widespread in consumer devices, are important scientific tools for diagnosing charged particle beams, short-wavelength photons, and non-neutral plasmas. Despite decades of use, however, some important aspects of the physics of phosphors remain topics of debate and investigation; depending on the material, this may include the structure of luminescence centers, the excitation and relaxation pathways, and/or the origin of the “dead voltage”[†]. Yet another question involving phosphors is a practical one; although they are routinely used for diagnosing both matter and antimatter systems, comparisons between the two are scarce.

Low-energy positrons incident on a phosphor screen have been found to produce significantly more luminescence than electrons do [1]. For two different wide-band-gap semiconductor phosphors (ZnS:Ag and ZnO:Zn), the luminescent response to a positron beam was compared with the response to an electron beam. For both phosphors, the positron response is significantly brighter than the electron response, by a factor that depends strongly on incident energy (0–5 keV). Positrons with just a few tens of eV of energy (for ZnS:Ag) or less (for ZnO:Zn) produce as much luminescence as is produced by electrons with several keV. We tentatively attribute this effect to valence band holes and excited electrons produced by positron annihilation and subsequent Auger processes.

These findings are expected to have significant utility for nonperturbatively diagnosing low-energy positron beams and plasmas (relevant to electron-positron pair plasma creation, antihydrogen experiments, slow positron scattering processes, and positronium ionization studies, among other applications). They potentially also represent a new approach for addressing longstanding questions about luminescent materials.

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[†] For most phosphors, no luminescence is observed when incident electrons' kinetic energy is below some threshold, which is usually orders of magnitude larger than the material's band gap. The transition to the linear regime, in which an increase in electron beam energy produces a proportional increase in the number of photons produced, may not occur until the energy exceeds several keV.

HfNbTaTiZr complex concentrated alloys, their microstructure and positron characteristics

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Studying complex concentrated alloys (CCAs; also often called high entropy alloys) [1] is very popular at present. The equiatomic, refractory alloy HfNbTaTiZr [2] belongs to this class and was devised for high temperature and biocompatible applications. This alloy exhibits the bcc structure at high temperatures due to the fact that all constituting elements show the bcc structure at such temperatures, and have very similar metallic radii (and thus easily mix). High configurational entropy is not needed to explain single, bcc phase of HfNbTaTiZr at high temperatures (even if high entropy contributes to the alloy stability, as does the mixing enthalpy). Upon cooling, there is a strong tendency to local order [3], which lowers the entropy, and eventually the alloy separates into two, hcp and bcc, phases with non-equiatomic compositions [4].

Since the understanding of any material has to rely on its microstructure, we proceed in this direction and simulate various structure-related properties of the HfNbTaTiZr alloy. An attempt is undertaken to simulate phase separated HfNbTaTiZr system, following the idea of phase transition in ZrNb alloys where the transition from bcc to hcp phase occurs when cooled [5], using the general geometrical relationship of these two phases [4,6]. It is also explained why the studied alloy cannot have a single, hcp structure, which might look natural since Hf, Nb, and Zr (making thus atomically 60 % of the alloy) are hexagonal (hcp) at low temperatures. In the simulations a pseudopotential code based on the density functional theory was employed.

Positron characteristics, such as the lifetime and affinity, of various alloys' configurations were also calculated, and we discuss what is possible to deduce from them in relation to the microstructure of the studied alloy. The role of unintentional impurities, like oxygen and nitrogen, is also examined.

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***Ab initio* study of the effect of molecular vibrations on the positron-binding to polyatomic molecules**

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The positron, which is the anti-particle of the electron, is now widely used in both scientific and technological areas. The detail mechanism of such processes, however, is still unclear in the molecular level. A positron affinity (PA) value, which is a binding energy of a positron to an atom or molecule, has now been experimentally measured by Surko and co-workers for many molecular species such as acetaldehyde, acetone, and acetonitrile molecules [1], based on the vibrational Feshbach resonance by incident low-energy positrons. Thus, in order to elucidate the mechanism of the positron binding to molecules, the theoretical analysis including the effect of molecular vibrations is indispensable. In this study, we will show the effect of molecular vibrations on PA values, based on *ab initio* multi-component quantum Monte Carlo (QMC) [2] and molecular orbital (MCMO) [3] methods for the electronic and positronic wave functions simultaneously, and the anharmonic vibrational quantum Monte Carlo (QMC) method [4].

In order to analyze the PA value including the effect of molecular vibrations, we introduced vibrational averaged PA (PA_v) defined by the following equation:

$$PA_v \equiv \frac{\int PA^{[X]}(\mathbf{Q})|\Psi_v(\mathbf{Q})|^2 d\mathbf{Q}}{\int |\Psi_v(\mathbf{Q})|^2 d\mathbf{Q}},$$

where \mathbf{Q} is a set of vibrational coordinates and Ψ_v is the vibrational wave function of the v -th vibrational excited state. The $PA^{[X]}(\mathbf{Q})$ is the vertical PA value at the molecular geometry \mathbf{Q} , defined by the total energy difference of the parent molecule (X) and its positron attached system ($[X; e^+]$) as $PA^{[X]}(\mathbf{Q}) \equiv E^{[X]}(\mathbf{Q}) - E^{[X; e^+]}(\mathbf{Q})$. In this study, $E^{[X; e^+]}(\mathbf{Q})$ and $\Psi_v(\mathbf{Q})$ were calculated with configuration interaction level of MCMO theory [3] and vibrational QMC method [4], respectively.

In the case of formaldehyde (CH_2O) molecule, the vertical PA value at the equilibrium position is predicted as +25(3) meV with QMC calculation. Applying the anharmonic vibrational analysis, the vibrational excitation of the C=O stretching mode enhances the PA value, whereas the excitation of CH_2 rocking mode deenhances it. We confirmed that such PA variations arise from the change in both permanent dipole moment and dipole-polarizability at each vibrational excited state. We will show some results of other larger molecules.

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Calculation of positron states and annihilation parameters in gamma and amorphous Al₂O₃

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Gallium nitride and related compounds attract much attention because of their applicability not only in light-emitting devices but also in power devices. The quality of gate insulator material plays a crucial role for the device performance and Al₂O₃ is a promising candidate. Recently, we applied slow positron beams in characterizing gate-stack Al₂O₃ layers [1]. It is thought that deposited Al₂O₃ layers have various structures depending on the preparation method and condition. In the present study, we construct appropriate structural models of gamma and amorphous Al₂O₃, which are often observed in real cases, and calculate positron states and annihilation parameters therein.

Gamma Al₂O₃ has a defect cubic spinel structure. To obtain a stoichiometric Al₂O₃, three cubic cells are needed. By removing 8 Al atoms, a stoichiometric Al₆₄O₉₆ structure is constructed. There are two different crystallographic Al sites in the cubic spinel structure, the octahedral (*O*) and tetrahedral (*T*) sites. Randomly removing 8 Al atoms from the *O* sites only or from both the *O* and *T* sites, we construct 16 different structural models and calculate positron states and annihilation parameters. Figure 1 represents the calculated positron annihilation parameters and examples of the positron density distribution. Depending on the local structure, the obtained annihilation parameters differ slightly. The calculated positron lifetime values fall in the same range as the experimental results [1].

Amorphous Al₂O₃ structures are modeled by first-principles molecular dynamics using cubic cells containing 160 atoms therein with various lattice parameters. Positron annihilation parameters are obtained as a function of the density and systematic correlations are observed.

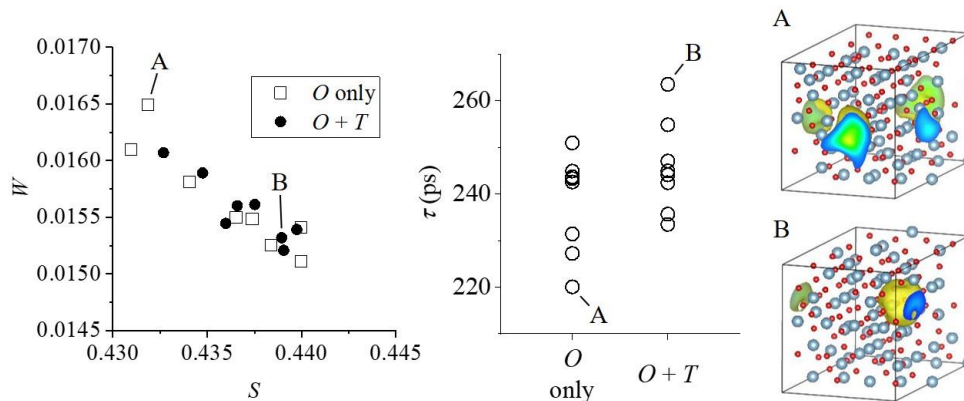


Figure 1 Calculated positron annihilation parameters and examples of positron density distribution (corresponding to the parameters marked “A” and “B”) in gamma Al₂O₃.

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Porous Metal-Organic Framework Glasses

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The last two decades has seen intensive research into developing metal-organic framework (MOF) materials in which the pore size and architecture can be specifically tailored by the assembly of metal co-ordinates together with rigid organic ligands. Many of the applications for MOFs include separation, gas adsorption, water purification [1]. The ability to control the positioning and growth of these materials into devices [2], membranes and sensors [3] is currently the focus of our research.

We have recently been characterizing porous glass MOFs in which a crystalline MOF is melt-quenched (MQ) to produce an amorphous glass [4-5]. MQ glasses are formed by quenching a liquid from above the melting temperature to below the glass transition temperature at a rate fast enough to avoid crystallization. Being able to retain and control the porosity of these highly novel materials is key to future applications. Positron Annihilation Lifetime Spectroscopy has been at the forefront of precisely measuring pore sizes and distributions. Here we present the latest results on glassy materials and potential future applications [4-5].

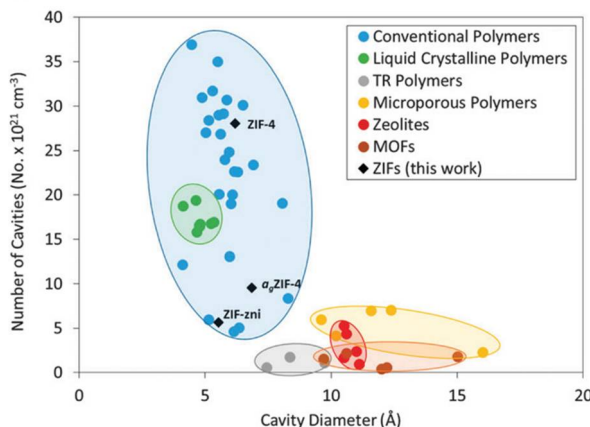


Figure 1 Comparison of PALS results for a range of materials including glassy MOFs [4].

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Current status of the AIST slow positron facility

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The AIST (National Institute of Advanced Industrial Science and Technology) slow positron facility provides an intense slow positron beam generated by an electron LINAC. The positron beam is mainly used for materials research employing positron annihilation lifetime spectroscopy (PALS). To date, two beamlines have been installed: one is used for the standard PALS measurement with an energy-variable beam (1 - 30 keV) [1], while the second is used for the Positron Probe MicroAnalyzer (PPMA). The PPMA enables us to perform two-dimensional mapping of positron lifetime with micrometer spatial resolution ($<100\mu\text{m}$) [2] and PALS measurements under atmospheric environment [3]. Both systems are arranged vertically to the ground, thus allowing the measurement of not only solid samples but also liquid and powder samples. The facility is open to external users through the "Nanotechnology Platform" project in Japan [4].

Recently, a new beamline was constructed to be compatible with new experimental fields. A coincidence Doppler broadening (CDB) measurement system and a buffer-gas trap, which can output nano-second positron bursts, will be developed with this beamline. The latter will be employed to demonstrate new positron experiments synchronized with laser sources.

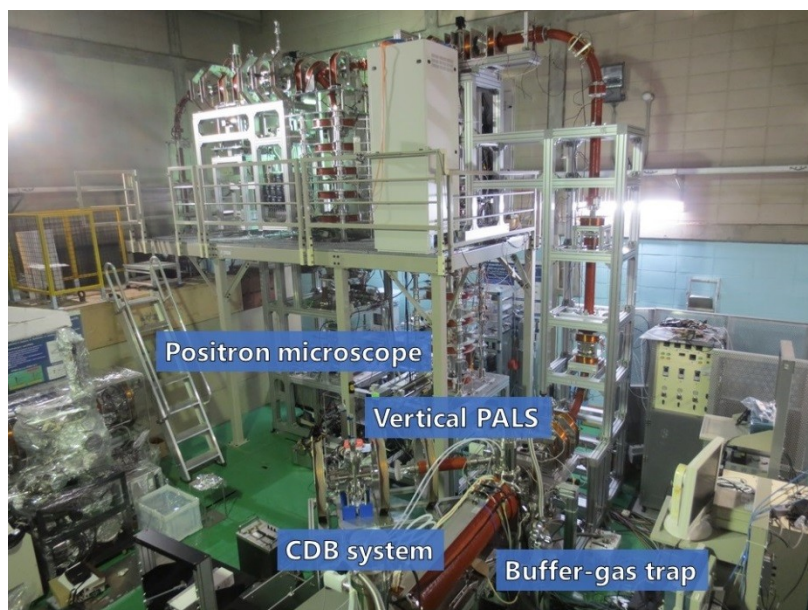


Figure 1 Overview of the slow positron facility at AIST.

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Development of Fast Plastic Scintillators for Positron Annihilation Lifetime Spectroscopy

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Jagiellonian Positron Emission Tomograph (J-PET) is a PET scanner based on plastic scintillators [1, 2, 3]. The aim of the J-PET Collaboration is to build a modular, light and portable PET scanner for the total body examination. Currently we are building prototype modules consisting of 1000 mm long plastic scintillator strips with silicon photomultipliers coupled at both ends [4].

Result of styrene and vinyltoluene polymerization will be presented. The time-temperature cycles were established for polymerization in small cylinders as well as for polymerization in the glass mold allowing to manufacture long plastic scintillator strips. A new method developed for the fast quality control of plastic scintillator strips was successfully applied during J-PET prototype building and will be introduced. The new scintillator was manufactured via bulk polymerization of vinyltoluene and the optimal concentration of the 2-(4-styrylphenyl)benzoxazole wavelength shifter [5]. The light yield for the best sample was established to be equal 10 000 photons per MeV. Obtained plastic scintillators were optimized for short rise and decay times needed in time of flight PET and PALS detectors. The rise time and decay time of the developed plastic scintillator were determined to be 0.5 ns and 1.9 ns, respectively.

J-PET is a multi-purpose detector designed for medical imaging and for studies of properties of positronium atoms in porous matter and in living organisms [6]. The obtained results prove that J-PET is capable of performing simultaneous imaging of the density distribution of annihilation points as well as positron annihilation lifetime spectroscopy [7]. Possibility of performing the three gamma photons imaging based on ortho-positronium annihilation, as well as the possibility of positronium mean lifetime imaging with the J-PET tomograph constructed from plastic scintillators will be also explored [6].

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On the reconstruction of defect depth profiles obtained from the positron annihilation experiment and chemical etching

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It is generally accepted that the positron beam technique allows to distinguish information about the depth distribution of defects or positron traps, which is extended below the entrance surface. However, the depth range of the examined defect distribution is limited to the depth of implanted positrons, which is about 1-2 micrometers. In turn, an experimental technique based on sequential etching of the tested sample does not have such a limitation and allows to recognize the distribution to a depth of about one hundred micrometres or more. In this case, conventional positron techniques based on ^{22}Na positrons are used, but we should stress that this is a destructive technique. Recently, this technique has been successfully used to study defects induced by implantation of heavy ions to a depth of approximately 10 μm . This encourages us to try to reproduce the distribution of real depths, e.g. the average lifetime of positrons in the samples tested. Mathematical considerations have allowed us to find useful relationships that can be used to recognize the actual distribution of the mean positron lifetime or shape of annihilation line, i.e., S-parameter, and thus to deduce the depth distribution of defects using the measured values. Our recent studies of pure Bi or Si implanted with Xe^{26+} illustrate the use of these relationships [1]. The main conclusion is that the defect concentration remains almost constant throughout the implanted layer, which is contrary to the theoretical predictions of the SRIM code. This suggests that not only nuclear collisions of implanted ions are responsible for the generation of defects, but also other processes.

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Sensitivity of nuclear emulsions to low-energy positrons

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In this work a new study of the sensitivity of nuclear emulsions to low-energy positrons is presented. Since more than a century, nuclear emulsions are an efficient instrument for charged particles tracking in high energy physics experiments. Nowadays their contribution remains fundamental, especially in those experiments where high spatial resolution is needed. Recently, thanks to their unmatched position resolution they were successfully employed in a positron interferometry experiment, where a submicron resolution was required. Emulsions are composed of silver bromide (AgBr) mixed with a gel in a 1:1 ratio and were specially prepared without the standard protective layer. On the other hand, positrons are produced by the b^+ decays of a ^{22}Na source, moderated by a tungsten thin film at about 2 eV energy and finally guided and accelerated in a purely electrostatic variable energy beam. The beam energy range used in this work is between 0.2 keV and 17 keV. The experiment makes use of the positron beam facility of the L-NESS laboratory in Como. The work starts from the preparation of the emulsions by mixing the sensitive AgBr grains of 200 nm in diameter with a gel that allows spreading the mixture on glass substrates of $5 \times 5 \text{ cm}^2$. Subsequently, the emulsions were exposed at different positron energies. After the expositions, the emulsions were developed to take a digital tridimensional grains reconstruction of the optical images. From the data analysis, it is possible to discriminate the signal from noise. The results clearly indicate that emulsions are sensitive to the positron beam, even at energies lower than 1 keV.

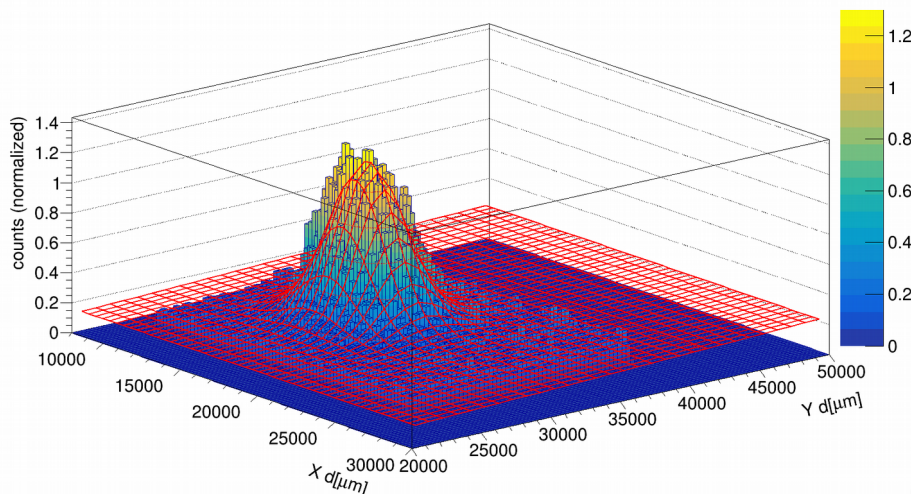


Figure 1. Example of 1 keV positrons detected with a nuclear emulsion.

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Determination of the Vacancy Formation Enthalpy Revisited by Temperature Dependent Doppler-Broadening Spectroscopy

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The coincident Doppler broadening spectrometer (CDBS) at the positron beam facility NEPOMUC of the research neutron source FRM II enables both spatially resolved defect studies and temperature dependent measurements by using Doppler broadening spectroscopy (DBS) of the positron-electron annihilation line. In order to investigate the near-surface region and the bulk of a sample, the positron implantation energy can be varied between 0.1 and 30 keV. The lateral resolution could be improved to below 50 μm by using an additional transmission positron remoderator inside the spectrometer [1]. Compared to conventional positron annihilation spectroscopy with ^{22}Na sources a further advantage of DBS using a positron beam is that no correction of the so-called source component is needed. With a heatable sample holder temperature dependent in-situ defect spectroscopy can be performed from room temperature up to 1000 K.

Since several decades, positron annihilation spectroscopy is known as powerful tool for the determination of vacancy formation enthalpy due to the unique sensitivity of positrons to open volume defects. Within this study the vacancy formation enthalpy of La (and Cu as reference material) was determined for the first time by temperature dependent DBS. Due to the high reactivity of the La surface all preparation was made under protective gas atmosphere. First, the as-received samples were annealed in situ, i.e. the decrease of the S-parameter indicated the annealing of lattice defects. During a second heating cycle the increase of the vacancy concentration was clearly observed from which the vacancy formation enthalpy could be calculated. In addition, a significant temperature dependence of the vacancy formation enthalpy in La was observed.

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The pulsed low energy positron system PLEPS: applications and new developments

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The pulsed low energy positron system PLEPS [1] is a user facility for defect depth-profiling with positron lifetime measurements using a monochromatic pulsed beam of variable implantation energy at the intense positron source NEPOMUC at the MLZ in Garching, Germany [2].

At present it is possible to measure with PLEPS positron lifetime spectra in the energy range between 0.5 keV and 20 keV with acquisition-rates between 10000-20000 counts per second, depending on the sample. It takes typically a few minutes to measure a lifetime spectrum with 4×10^6 counts at a single energy. A full depth-profile with 10-15 energies requires about 1-2 hours. Depending on the detector, an overall time-resolution of 180 ps-240 ps and peak-to-background ratios of up to 1.5×10^5 can now be routinely achieved within a time-window of 40 ns [3]. For precise measurements of long lifetimes (> 5 ns) it is now possible to extend the time window to 160 ns at an overall time resolution of 300 ps. The sample temperature can be varied between 80 K and 600 K.

Typical applications of PLEPS comprise the defect identification in thin layers and layered structures of semiconductors [4,5] and insulators [6], the investigation of irradiation induced defects in materials for fusion and fission, as well as the characterization of open volumes in glasses [7], polymers, polymer- and membrane layers [8]. In this talk we will describe the present setup of PLEPS and its performance, show some exemplary applications and give an outlook of future developments.

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Total Reflection High-Energy Positron Diffractometer at NEPOMUC

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Total Reflection High-Energy Positron Diffraction (TRHEPD) has been established as an ideal technique to determine the atomic positions of the topmost and immediate subsurface crystalline structure with highest accuracy [1]. Recently, the precise structure of the rutile-TiO₂ (110)-1x2 reconstructed surface - which has been under debate over the past 30 years - has been uncovered with the aid of TRHEPD [2]. Novel materials such as topological insulators or 2D materials can be investigated to determine not only the surface structure, but also the substrate spacing and potential buckling [3]. Moreover, the new approach of azimuthal analysis of the diffraction pattern might enable an even better separation of the signal that stems from different subsurface layers. However, up to now, there is just one TRHEPD setup available worldwide, which is located at the Slow Positron Facility (SPF) at the accelerator KEK in Japan.

We developed a new positron diffractometer coupled to the high-intensity positron source NEPOMUC at the research reactor FRM II in Munich. For the TRHEPD experiments, we plan to use the continuous, remoderated NEPOMUC beam, which has an intensity of $\sim 5 \cdot 10^7$ e⁺/s. The setup features an additional transmission-type remoderator using a 100nm thin Ni (100) foil to optionally further enhance the brightness. After the e⁺ beam passes a magnetic field termination, it is electrostatically focused and accelerated up to 30keV energy (25keV for the twofold remoderated beam). We simulated the e⁺ trajectories to optimize the system for different beam energies and for both, remoderated and twofold remoderated beam. The simulation for the focus onto the remoderator foil is shown in figure 1. After the twofold remoderation, we expect a slightly converging beam with a diameter of ~ 1 mm on the MCP. The characterization of the e⁺ beam and first experimental results are expected for summer 2019.

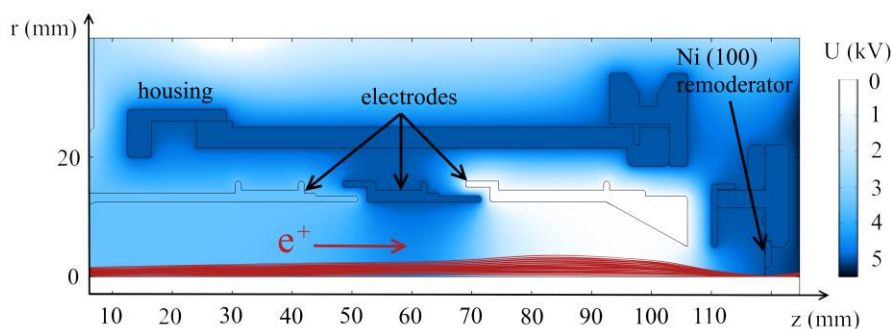


Figure 1
Simulation of the positron beam, that is focused onto the remoderator foil.

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Upgrade of the NEPOMUC re-moderator

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The neutron-induced positron source Munich (NEPOMUC) provides a monochromatic low-energy positron beam with an intensity of $> 1 \cdot 10^9$ e⁺/s [1] and a full width at half maximum (FWHM) diameter of about 10 mm. To create a small beam focus or sharp positron pulses of 100 ps FWHM the beam brightness needs to be enhanced by re-moderation. This is achieved by focusing the primary beam magnetically on a tungsten single crystal W(100) in reflection geometry. Afterwards the beam exhibits an intensity of $> 3 \cdot 10^7$ e⁺/s and a diameter of less than 2 mm (FWHM) [2].

Based on the experiences with the remoderator setup, we redesigned and extended the existing construction to further optimize the beam quality with respect to intensity and beam brightness. The new design allows a replacement of the remoderator crystal within several minutes and without breaking the beamline vacuum. It enables, therefore, a systematic test of different remoderator materials. Additionally, it is possible to clean and anneal the crystal surface by heating in-situ through electric current. The new crystal holder system permits to move the remoderator with high accuracy in micrometer steps, which allows a positioning of the crystal surface precisely in the focus of the magnetic lens, resulting in an increase of the beam brightness. In addition, a fine metering valve can be used to treat the crystal surface with different gasses, e.g. atomic hydrogen or oxygen.

With the remoderator upgrade it was possible to increase the re-moderation efficiency and to raise both, the brightness and intensity of the remoderated NEPOMUC beam. The effects of the higher beam quality have been already detected in positron annihilation lifetime spectra obtained with the Pulsed Low-Energy Positron System PLEPS [3]. Here, the new setup leads to sharper pulses of ≤ 100 ps and a consequently better overall time resolution at higher beam intensities. Moreover, from the increase of the brightness also other applications benefit, e.g. the Coincidence Doppler-broadening Spectrometer [4] or the Scanning Positron Microscope [5], where the excellent phase space quality of the re-moderated beam is crucial for timing and a high spatial resolution. The increased beam intensity will further reduce the measurement time of all instruments. Additionally, we will present results of selected materials, which we have investigated with respect to their re-moderation properties.

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Digital positron annihilation lifetime spectroscopy for applications with high count rates

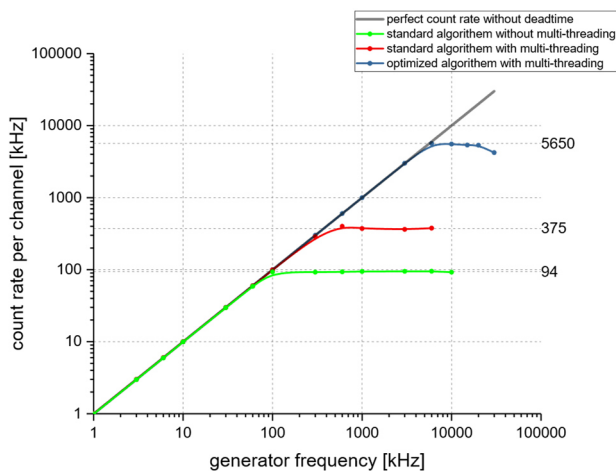
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For over 10 years[1] of research the positron group from the MLU Halle and the HZDR are developing a solution to employ a digital positron lifetime setup at the MePS[2] system at the ELBE[3] accelerator, using an appropriate digitizer to replace the analog setup. The idea is to analyze data online using a software written in C++ and a graphical user interface designed in QT. Over the years, a conventional setup could be built up and tested using an *Agilent* digitizer with an inhouse made coincidence trigger unit, which significantly reduces the data traffic. Unfortunately, the bandwidth limitation of this digitizer was too high to use the same technique at the MePS system, because this setup reaches up to 100 kcps at optimal setting and highest bunch repetition rates. To overcome this problem a new generation of digitizer (Teledyne SPDevices ADQ14DC-2X) was tested using an innovative FPGA supported pulse detection firmware. This firmware reduces the transferred data stream to the pulse shape only, coupled with an appropriate timestamp. Based on the data reduction an inhouse made software was written to calculate the time stamps for the positron generated PMT pulses and the 3.2 MHz ELBE time reference signals online.



In this talk the hard- and software solution will be presented. The used FPGA based pulse detection logic, the drastically simplified time calculating algorithm and the multithreading approach, which leads to a maximized throughput for high performance positron annihilation lifetime spectrometers will be shown in detail.

Figure 1 A generator pulse is used for start and stop to check the limitation of the used software changes: (grey) perfect performance without dead time, (green) standard algorithm, (red) standard algorithm with multi-threading and (blue) simplified algorithm with multi-threading

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Optimized High-speed digitizers for slow positron applications

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This talk presents the latest available technologies developed by Teledyne SP Devices in the field of high-speed digitizers for generic physic application, and focus on specific requirements discussed in the area of slow positron high performance DAQ with special attention to the high resolution & high speed ADC techniques, the embedded real-time pulse detection & data reduction capabilities, and the data throughput optimization for continuous, streamed data transfer to host PC.

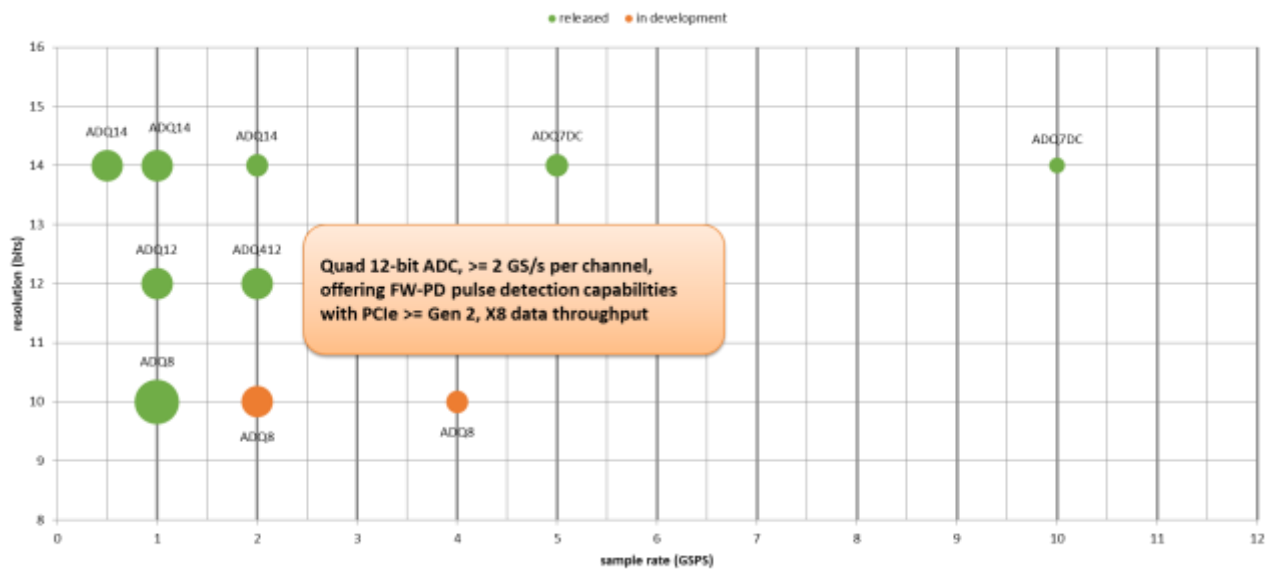


Figure 1 Optimal digitizer product portfolio for slow positron applications

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Status of the Positron Sources at the Superconducting Electron LINAC ELBE

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The Helmholtz-Center Dresden-Rossendorf operates several user beamlines for materials research using positron annihilation energy and lifetime spectroscopy. The superconducting electron LINAC ELBE [1] serves as a driver for hard X-ray production from electron-bremsstrahlung, which in turn generates positrons through pair production. **GiPS**, the Gamma-induced Positron Source directly generates electron-positron pairs inside the sample under investigation [2]. The source is especially suited for materials, which are not qualified for vacuum conditions or because they impose hazards or intrinsic radioactivity.

MePS, the Mono-energetic Positron Source utilizes positrons with fixed kinetic energies ranging from 500 eV to 18 keV [3] for thin film studies, which allows depth profiling. A magnetic beam transport system guides positrons passing on the way chopping, bunching, and accelerator sections to the samples under investigation. The simultaneous operation of chopping and bunching techniques supported by digital acquisition generates nearly background and distortions free spectra as well as offers timing resolution down to about 210 ps.

The **MePS** facility is currently complemented by additional beamline **AIDA-II** - Apparatus for In-situ Defect Analysis - where defect investigations can be performed *in-situ* in a wide temperature range during thin film growth and under ion irradiation. To further improve timing resolution additional $\lambda/4$ buncher has been recently installed and commissioned. Complimentary, functionally similar setup, **AIDA-I** [4], is in operation at a ²²Na-based mono-energetic continuous positron beam [5] used for *in-situ* Doppler-broadening positron annihilation spectroscopy experiments.

Recent developments at all beam lines as well as some exemplary experiments will be presented.

The **MePS** facility has partly been funded by the Federal Ministry of Education and Research (BMBF) with the grant PosiAnalyse (05K2013). The initial **AIDA** system was funded by the Impulse- und Networking fund of the Helmholtz-Association (FKZ VH-VI-442 Memriox). The **AIDA** facility was funded through the Helmholtz Energy Materials Characterization Platform.

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Polarized positron beam developments

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High intensity polarized positron beams are of particular interest for applied and fundamental physics research [1], investigating the structure of matter from the macroscopic molecular scale down to the elementary scale of quarks and gluons. Since the experimental demonstration [2] of the PEPPo production of polarized positrons (Fig. 1), electron linear accelerators of moderate energies (5-100 MeV) offer the possibility to produce highly polarized positron beams whose polarization and flux is limited only by the technological capabilities of the initial polarized electron source.

Building on these results, several projects are currently developing at the Continuous Electron Beam Accelerator Facility (CEBAF) of the Thomas Jefferson National Accelerator Facility (TJNAF) in Newport News (VA, USA) and the ALTO (Accélérateur Linéaire et Tandem à Orsay) facility in Orsay (France). This presentation will discuss the actual status of these projects and the latest technological developments for a PEPPo based polarized positron source.

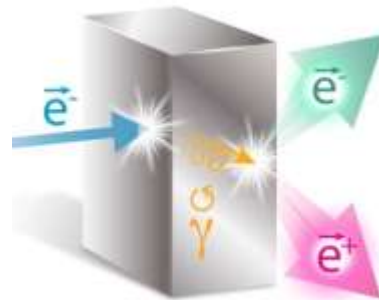


Figure 1 Schematic of the principle of operation of the PEPPo technique.

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Do we need a mono-energetic spin-polarized positron beam?

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In the framework of the Helmholtz national roadmap for large scientific infrastructures, the Helmholtz-Zentrum Dresden-Rossendorf [1] plans a significant upgrade of the existing ELBE center for high-power radiation sources. The new facility DALI (Dresden Advanced Light Infrastructure) will feature an increased number of beam lines dedicated to super-radiant coherent THz radiation [2] with high repetition rates and high intensities. Various applications in solid-state physics, biological systems, and material sciences are envisioned which will focus on fs-resolution pump-probe techniques, angular-resolved photoelectron spectroscopy, high-pressure cells, and in-situ bio-sample handling.

Additionally, the available intense electron beam (50 MeV energy, 2 mA average current) with MHz repetition rates serves as a driver for intense secondary positron sources thus extending the available positron beam intensity beyond the existing MePS (Mono-energetic Positron Source) installation [3]. Besides a high-intensity positron source for depth-resolved positron annihilation lifetime spectroscopy studies, a spin-polarized mono-energetic positron beam could be realized which would open a new field of applications for electron-spin sensitive studies.

With Helmholtz' mission in mind to serve the (inter-)national scientific community with large scale infrastructures for the advancement of science, the focus is now on the feasibility of such an installation and scientific visions of the communities justifying the effort of realizing such a project. Pioneering work by the BEPPO collaboration at the Thomas-Jefferson National Accelerator Facility (TJNAF) on polarized positron production from an energetic spin-polarized electron beam [4] demonstrated the proof-of-concept of spin-transfer up to 82%. However, the high-repetition rate DC photo-injector at TJNAF features only a small electron bunch charge and a new source for nC of spin-polarized electrons with repetition rates of 1 MHz has to be developed.

In the contribution, we will discuss possible spin-related phenomena ranging from surface magnetism as shown in [5,6], defect related magnetism and predictions of spin-dependent annihilation lifetimes [7].

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Positron burst detecting array system based on SiPM and DRS4

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The timing resolution of positron lifetime detector is usually based on BaF₂ scintillator and quartz window fast PMT [1]. The limitation of this design lies in BaF₂'s low fast component light output and low stopping power, as well as PMT's limited quantum efficiency and time jitter. Therefore, the timing resolution of traditional positron annihilation lifetime measuring system is difficult to be further improved.

In the work, we proposed a new positron annihilation lifetime spectrum measuring method. The spatially arranged positron burst detecting system is based on state of the art LYSO crystal and silicon photomultiplier (SiPM) array, readout by multichannel fast waveform digitizing chip DRS4[2], to obtain high sensitivity and better timing resolution at the same time. Current system has 32 detector modules. Each module is composed by 64 3mm × 3mm × 5mm LYSO crystals coupling to 64-channel 3mm × 3mm SiPMs array. All timing signals from a detector are digitalized by two 32-channel high speed sampling board based on DRS4 chip, and then implemented digital timing by PC, instead of traditional leading edge or constant fraction discriminator circuit. With buncher signal used as starting trigger and each channel's timing signal as stopping signal, the time spread distribution would be the lifetime spectrum of positron.

The single channel detector performance was investigated and optimized by improvement of LYSO scintillation light collection, SiPM readout and temperature stability. Preliminary results showed that the double 511keV coincidence timing resolution of two single channel detectors achieved 84 ps, measured by placing a Na²² source in the middle. Module level and system level studies are being carried out.

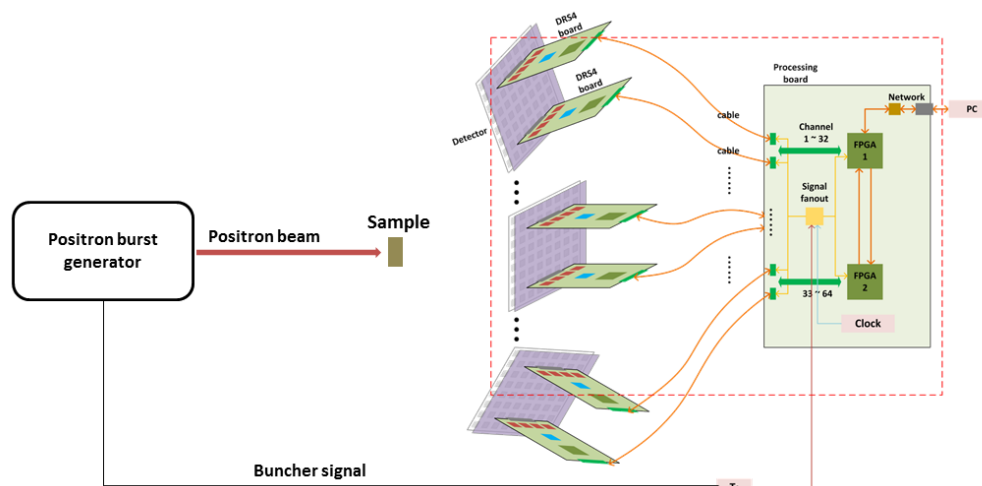


Figure 1 Schematic of the positron burst detecting array system

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The new operational Slow POsitrone faciLiTy in Israel: SPOT-IL

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The Slow POsitrone faciLiTy in Israel (SPOT-IL), located at the Hebrew University of Jerusalem, is now operational. The SPOT-IL beam follows a traditional design [1], using a ²²Na source, ~40mCi [2]. A tungsten foil moderator was annealed prior to its mounting on the source capsule. A compact new design of the source shielding allowed convenient positioning of the source onto the moderator. A grounded target cell allows sample changing without breaking the beam-line vacuum and is designed to allow a combined measurement of sample conductivity and Doppler Broadening (DB), with the flexibility to add more detection options in the future, such as low temperature for integrated in-situ electronic measurements. The detection system is comprised of HPGe and BaF₂ detectors, facing each other, for low background DB measurements.

The successful operation of the beam was proven by a controlled positron beam spot seen on an MCP phosphor screen, located at the beam-dump position, and by the detection of the 511 keV annihilation peak when a Perspex sample was positioned in the beam in front of the detectors.

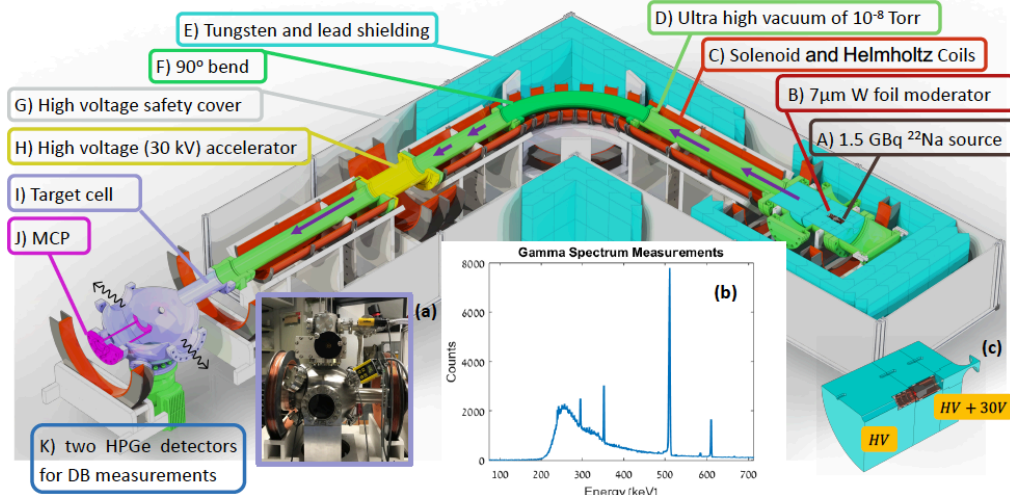


Figure 1 A model section view of SPOT-IL. (a) The target cell. (b) A γ spectrum (HPGe), with a peak of 8000 counts at 511 keV (c) Section view of the source shielding with the pre-accelerator.

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The role of vacancies and hydrogen in the photochromism of YO_xH_y thin films examined by in-situ Positron Annihilation Spectroscopy and μ SR

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Yttrium oxyhydride (YO_xH_y) is a promising mixed-anion material in view of its special photochromic properties, offering prospects for application in smart windows [1]. Doppler Broadening Positron Annihilation Spectroscopy (DB-PAS) depth profiling was applied to probe the electronic structure and the evolution of vacancies in YO_xH_y thin films and related materials. A strong systematic variation in the S- and W-parameters of Y, $YH_{1.9+\delta}$, YO_xH_y and Y_2O_3 thin films is observed, caused by distinct differences in their electronic structure that spans the range from metals to a large band gap insulator [2]. Positron Annihilation Lifetime Spectroscopy (PALS) reveals the presence of vacancies and positronium formation in the YO_xH_y films. In-situ optical illumination of the semiconducting YO_xH_y films above the band gap leads to an increase in S-parameter, plausibly induced by the generation of vacancies or growth into small vacancy clusters [2]. Intriguingly, the S-parameter does not relax during optical bleaching under dark conditions, indicating persistent local rearrangements of vacancies and hydrogen ions.

Furthermore, low-energy Muon Spin Rotation (μ SR) experiments on $YH_{1.9+\delta}$ and YO_xH_y thin films indicates the formation of μ^+H pairs at tetrahedral sites. In-situ illumination of YO_xH_y films leads to a clear reduction in muonium formation, that could be affected by photo-excitation of charge carriers during photochromic darkening, relaxing slowly upon bleaching.

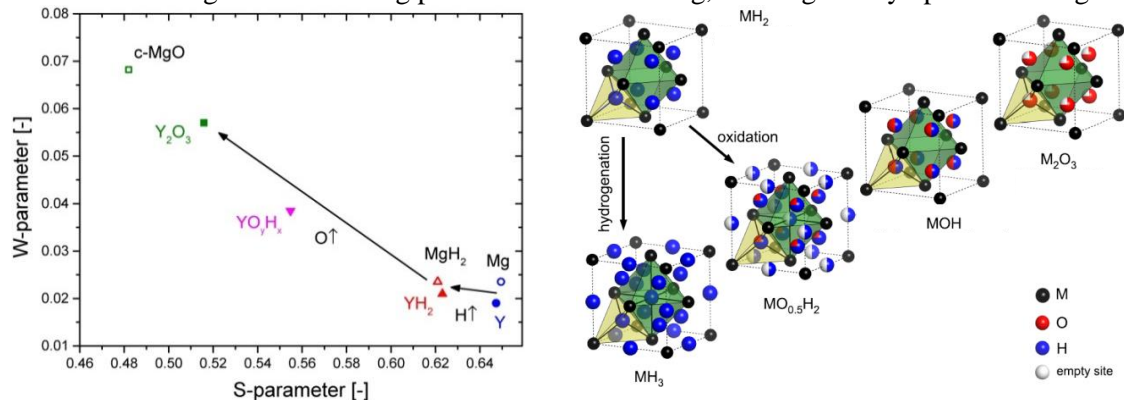


Figure 1 (a) S-W diagram (best-fit values) for Y, $YH_{1.9+\delta}$, YO_xH_y and Y_2O_3 thin films [2], (b) Schematic crystal structures of rare-earth oxyhydrides with different H^-/M and O^{2-}/M ratios [3].

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Variable energy positron annihilation lifetime spectroscopy studies of perovskite oxide electronic materials

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The potential of ABO_3 materials for electronic applications has been long recognized due the diverse range of electron properties exhibited by otherwise structural similar materials [1]. The discovery that a two dimensional electron gas can form at the interface between, for example $SrTiO_3$ and $LaAlO_3$ has accelerated this interest [2]. More recently, the realization that the transparent perovskite oxide $BaSnO_3$ can exhibit excellent conductivities has further extended the possible applications range for these materials [3]. Here we report positron annihilation lifetime measurements (PALS) and supporting density function theory (DFT) calculations on two perovskite materials lanthanum aluminate, $LaAlO_3$ and barium stannite $BaSnO_3$.

It has been difficult to grow $LaAlO_3$ thin films of sufficient thickness to enable characterization by VE-PAS methods, here we detail VE-PALS measurements 120 nm and 140 nm thick films grown by pulsed laser deposition, and on $LaAlO_3$ single crystal substrates. The results of DFT calculations, performed using Abinit, on positron lifetimes are also given.

Further, we report the results of VE-PALS measurements on $BaSnO_3$ films, both undoped and La-doped, grown by molecular beam epitaxy by two different groups. DFT calculated positron lifetime values for cation vacancy defects in barium stannite are reported. The relations between carrier concentration, dopant concentration and vacancy defect content inferred from PALS is discussed.

The PALS results and calculated positron lifetime values for $LaAlO_3$ and $BaSnO_3$ are compared to those obtained previously for the perovskite oxide titanates $SrTiO_3$ and $PbTiO_3$.

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Positron Annihilation studies of Various doped β -Ga₂O₃ Single Crystals with a Variable Energy Positron Beam

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Growth of Czochralski and vertical gradient freeze grown doped β -Ga₂O₃ (different doping levels of Zr, Mg) will be presented with support from theory [1]. Positron Annihilation Spectroscopy (PAS) were used to study vacancy, vacancy-donor pairs and clusters. β -Ga₂O₃ shows promise as an ultra-wide bandgap transparent semiconducting single crystalline material with n-type conductivity. UV/VIS/NIR optical spectroscopy was used to measure the bandgap and qualitatively compare free carrier concentration between crystals with varying concentrations of dopants. Hall effect, four-point contact current-voltage (I-V) and capacitance-voltage (C-V) measurements are used to measure electron mobility, carrier concentration, resistivity, and dopant activation energy.

Several possibilities for this deep level could be a deep acceptor such as gallium vacancies or Fe or Ir impurities (Fe and Ir have been observed with SIMS with no standards), or a deep donor such as an oxygen vacancy. Contact I-V measurements show a resistivity of down to 0.02 Ω -cm and an activation of 5-13 meV will be related to the positron results. Hall effect measurements show carrier density on the order of 10^{17} to 5×10^{18} cm⁻³ and a mobility of approaching 100 cm²/Vs [1]. The relationship between electron mobility and charge concentration was investigated with respect to vacancies through PAS. Samples throughout the crystal and melt were measured to understand how the growth process impacted the growth results. Tailoring the doping concentration and growth environment is the key to reducing the intrinsic defects and impurities and improving electron mobility within Zr:Ga₂O₃. Zirconium-doped β -Ga₂O₃ shows promise as a high free carrier concentration material with high mobility, requiring future work on reducing compensating defects.

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Depth-resolved porosity of subnanoporous silica films elucidated by the low-energy positron lifetime technique and in-situ FT-IR-ATR

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In order to improve the functionality of separation membranes, much efforts for controlling the nanoporosity have been made in both academia and industry. For a typical gas separation membrane, a several hundred nanometers thick active top layer, which separates target gas molecules, is formed on a porous support. Depth-sensitive evaluation of the pore structure in the near surface region is thus important to develop innovative separation membranes. In the present work, we applied variable-energy positron annihilation lifetime spectroscopy (VEPALS) and gas adsorption measurement using FT-IR-ATR (in-situ FT-IR-ATR) to evaluate the pore structure of silica-backed subnanoporous bilayer films fabricated on silicon wafers, in order to characterize the pore structure in the near surface region.

A subnanoporous bilayer silica film, consisting of a top-layer and base-layer with different refractive indices, and the corresponding monolayer silica films were fabricated on silicon wafers through plasma-enhanced chemical vapor deposition [1,2]. Table 1 shows the refractive index and thickness for the prepared silica films, obtained by spectroscopic ellipsometry.

The average pore size of the silica films was evaluated from the long-lived *ortho*-positronium (*o*-Ps) lifetime component using VEPALS. Fig. 1 shows typical VEPALS data measured at $E = 5$ keV for the present silica films. As shown in the figure, the long-lived *o*-Ps lifetime for the bilayer film agrees with that for the top film, significantly shorter than for the base film. This suggests that the pore sizes at the near-surface of the former films are consistent with each other, and smaller than for the latter film.

Details of the VEPALS and in-situ FT-IR-ATR results for the silica films will be discussed in the presentation.

Table 1 Refractive index and thickness for the present silica films

	Refractive index (630 nm)	Thickness [nm]
Top film	1.420	826
Base film	1.318	520
Bilayer film	1.355	1387

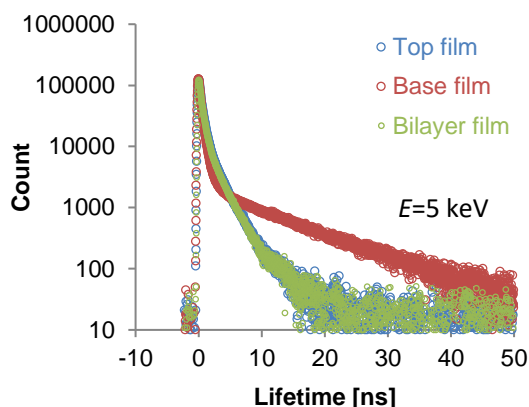


Figure 1 Positron annihilation lifetime data for the present silica films.

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Compensating defects in epitaxial Ge and Ge_xSn_{1-x}

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Increasing the carrier concentration in epitaxial Ge and GeSn above 10^{19} cm^{-3} poses a challenge from a defect point of view, as compensating defects are abundantly created in the growth of the layer. As the intent is to further increase the carrier concentration above 10^{20} cm^{-3} and semiconductor doping starts to resemble more alloying than traditional doping, we are entering unfamiliar territory when it comes to defect dynamics.

We have used positron annihilation spectroscopy (PAS) in combination with density functional theory (DFT) calculations to study compensating vacancy-donor complexes in epitaxial layers of Ge and GeSn doped with P and As. As expected the dopants form complexes with the native vacancy defects. In previous studies [1,2] both mono- and divacancy complexes have been observed in highly doped Ge. Whereas monovacancy complexes dominated in diffusion doped bulk Ge [1], divacancy complexes were observed in implanted and laser annealed Ge [2]. From the experimental results it is clear that monovacancies dominate the positron annihilation in all studied epitaxial layers. DFT calculations indicate that Sn does not have the desired effect of trapping vacancies, as the binding energies for V-Sn pairs is clearly lower than for complexes involving dopants. However, both experimental and computational PAS results indicate that Sn is having an impact on the annihilation state of the positrons.

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Positron annihilation in polyelectron system of strong spin-orbit field induced by bismuth impurity centers in natural silicon

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In silicon to be characterized by a low spin-orbit interaction, a heavy and oversized atom of bismuth impurity creates strong spin-orbit field which allows one to increase both the efficiency of spin polarization of charge carriers and energy of storing of information in the process of quantum computing. The tuning of qubit-forming Bi impurity centers of different symmetry is a challenging problem in manipulating the spin interactions. Meanwhile, a data on local electron properties of the crystal lattice, to be usually obtained with the positron probing, are lacking for Bi impurity centers. Having applied PALS and Hall effect measurements, for the first time we have observed a decrease of probability of 2γ -annihilation with the increase of number of electrons contacting positron at the bismuth impurity centers having both T_d and D_{3d} symmetry.

The transition of electrons from the conduction band to the donor ground state $E\{\text{Bi}\} = E_c - 0.069$ eV in the polyelectron system of Bi impurity center having T_d symmetry has been accompanied by an increase of the lifetime of e^+e^- pairs regarding 2γ -annihilation.

Enormously large cross-section of localization of positron is estimated to be equal to $\sim (1.3-1.7) \times 10^{-13}$ cm² with the growth of occupancy of the donor level, $\Delta n_e [E\{\text{Bi}\}] \sim 1.2 \cdot 10^{16}$ cm⁻³, with decreasing temperature from 295 to ~ 25 K. Involvement of ²⁹Si atom(s) tied to ²⁰⁹Bi one in the impurity center influences markedly on 2γ -annihilation of a localized positron. The averaged over temperature the probability of 2γ -decay per unit time becomes larger by a factor of $\Delta \sim 2.18$ compared to the value $\Gamma = (2.09 \pm 0.09) \times 10^9$ s⁻¹ known for the isolated polyelectron (e^+e^-) [1]. The picture looks as if the admixture of the charge-even states of e^+e^- pairs to the polyelectron in the spin-orbit field of Bi impurity center would decrease probability of its long-lived 2γ -decay, whereas the charge-odd states of e^+e^- pairs inhibit the contribution of short-lived component of the singlet e^+e^- pairs to the resulting probability of 2γ -annihilation.

Owing to trapping a vacancy, Bi donor center changes its symmetry to D_{3d} after irradiation of material with 15 MeV protons. The Bi atom saturates its valency, increases the number of bonds in the vacancy-Bi-atom pair (V-Bi), and the factor Δ decreases its value by $\sim 10-11\%$. The V-Bi pair is a deep donor that is seen from the data of electrical measurements in the course of isochronal annealing. Also, the polyelectron system formed in the spin-orbit field of V-Bi pair is thermally stable up to ~ 350 °C. Then the probability of 2γ -decay, $\Delta \times \Gamma$, begins restoring its value, and the Bi impurity center acquires T_d symmetry during a rather short annealing stage ranging temperatures 370 to ~ 430 °C. The effects observed are discussed in the light of current reconsidering of a whole conception of formation of the vacancy-phosphorus centers that trap positrons and are characterized by weak spin-orbit interaction in silicon [2-4].

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Electrical field-controlled ON-OFF ferromagnetism in metal oxide films

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In the context of Digital Agenda for Europe within the Horizon 2020 Programme, which stresses importance of energy efficiency, voltage control of magnetism is expected to realize ultra-low power magneto-electronics. Modern magneto-electronic devices are ultimately controlled by electric currents, inherently involving a significant energy loss by heat dissipation. Hence, even a partial substitution of electric currents by electric fields to manipulate such devices would already result in a remarkable energy saving [1]. Therefore, a stable, tunable, and non-volatile magneto-electric effect to tailor magnetism via electric fields is crucial for energy-efficient applications. The voltage-induced ionic motion (magneto-ionics) is attracting increasing interest driven by a possibility for an electrical modulation of magnetism to an extent never attained by any other magneto-electric coupling mechanisms [2]. We have recently investigated using positron annihilation spectroscopy and magnetometry techniques the electrolyte-gated and defect-mediated oxygen and cobalt migration in paramagnetic Co_3O_4 , which allows for voltage-controlled ON-OFF room temperature ferromagnetism [3]. A negative voltage reduces Co_3O_4 to Co (ferromagnetism: ON), resulting in a graded material including Co- to O-rich regions. A positive bias reverses the process oxidizing Co back to Co_3O_4 (paramagnetism: OFF) [Fig. 1a]. These gate-induced O and Co migration processes are driven by complex vacancies (clusters of cobalt and oxygen vacancies; see Fig. 1b), whereas O transport is in addition assisted by grain boundaries, which may act as diffusion channels and allow for an exceedingly large incorporation of oxygen. The steady states as a function of bias as well as kinetics of defect-assisted ion migration will be discussed in detail.

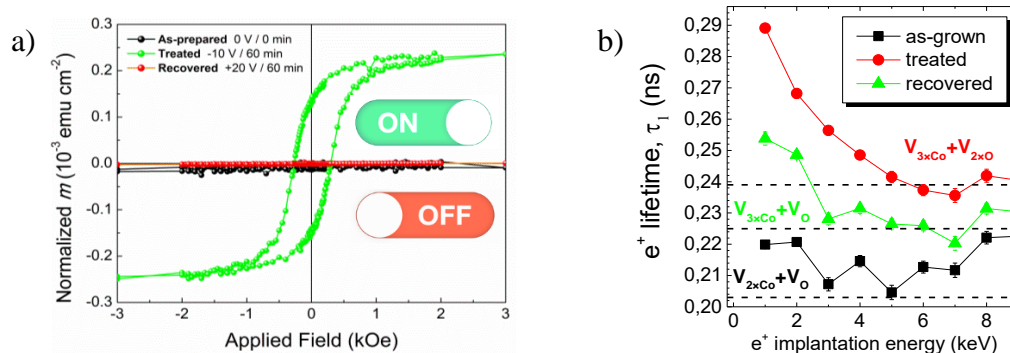


Figure 1 Electrical fields induced magnetic switching (a) and corresponding defect structures calculated by *ab-initio* DFT (b) for the as-grown, treated with a negative, and a positive bias Co_3O_4 films.

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Different curing strategies to create isolated pores in ultra-low-k thin films

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A slow annealing ramp (10 K/min.) during thermal curing of spin-on ultra-low-k (ULK) thin films generates enlargement of the pore size as a function of curing temperature. This phenomenon suggests porogen agglomeration during curing, which forms larger and linked pores extended up to the film surface as a consequence. Such a pore linking would likely increase the k value due to moisture or other impurities absorption and possibly could lower the mechanical stability. We propose to vary the curing ramping time up to the optimum curing temperature of 450 °C in order to immobilize porogen molecules and hinder their clustering, hence to prevent the creation of interconnected (open) pores. As a probe of porosity positron annihilation lifetime spectroscopy (MePS [1]) and Doppler broadening positron annihilation spectroscopy (AIDA [2]) have been utilized and results of different curing slow ramps (10-40K / min.) and for the so-called rapid curing (without any intentional ramp) will be shown. In Fig. 1 the annihilation line shape parameters S and W, and the $3\gamma/2\gamma$ ratio for the rapid and in-situ slow (10 K / min.) curing is presented. A smaller value of S and a wider plateau of W for positron energies below 6 keV for the rapid curing case suggest smaller pore size and different pore wall chemistry as well as more homogenous pore distribution, respectively. The latter is reflected in the $3\gamma/2\gamma$ ratio as the increased o-Ps escape probability for the rapid cured film.

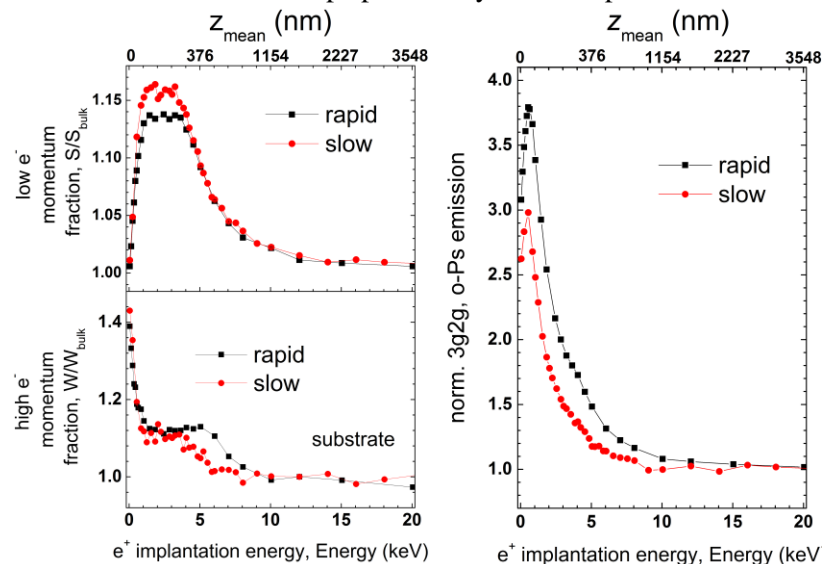


Figure 1 Normalized S and W-parameters and $3\gamma/2\gamma$ for the rapid and slow cured ULK films.

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The origin of the p-type conductivity in thin films of copper chromium delafossites deposited by Metal-Organic Chemical Vapor deposition investigated by Positron Annihilation Spectroscopy

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Commercially available transparent n-type semiconductors are characterized by electrical conductivities around 10^3Scm^{-1} and by transparencies up to 90% in the visible range. The quest for p-type semiconductors with similar properties has generated a strong interest in copper based delafossites CuMO_2 (where $M = \text{Al, Cr, B, Ga or In}$). Indeed, CuAlO_2 was the first reported p-type semiconductor with an acceptable level of optical transparency [1] and since then a record value for electrical p-type conductivity in Mg doped CuCrO_2 has been reported [2]. However, in order to optimize the optoelectronic properties of these materials, a good understanding of the origin of the p-type conductivity is required. Among the main candidates, the Cu vacancies [3] and O interstitials [4] have been suggested.

In this work, thin films of copper chromium delafossites deposited on Al_2O_3 substrates by the Metal-Organic Vapor Deposition method have been studied. In some instances, a subsequent thermal annealing at 900°C under the same gaseous conditions as during deposition was performed. Doppler Broadening Positron Annihilation Spectroscopy (DBPAS) measured with the slow positron beam developed at CEMHTI was then used to characterize these samples. The positron annihilation characteristics measured in the as-deposited films are seen to evolve upon annealing and this evolution is compared to results obtained by electrical measurements, X Ray Diffraction Spectroscopy, and Scanning Electron Microscopy. This combined approach allowed us to establish the origin of the p-type conductivity in these samples.

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Slow positron annihilation studies of black and reflective Al films prepared by magnetron sputtering

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In this work we present results of study of Al films prepared by pulsed DC magnetron sputtering: (i) smooth reflective Al films deposited in 0.5 Pa Ar atmosphere and (ii) rough black Al deposited in 0.5 Pa Ar + N₂ atmosphere. In case of reflective films the incident light is scattered into various angles. The total diffusion reflectance falls into range of 65 – 85 % depending on the film roughness and wavelength of the incident light. However in case of black films the incident light is absorbed in the film due to multiple light reflections from the surface resulting in a total diffusion reflectance 2 – 10 %.

AFM and TEM measurements revealed different structure of reflective and black Al films. Surface roughness of both types of films linearly increase with increasing film thickness. In reflective Al grains form compact film, while in black Al grains form porous moth-eye-like structure. The nano-porosity rather than the surface roughness is thus the key factor leading to the blackening of the films. In porous metals containing nano-cavities a thermalized positron may pick an electron on inner surface and escape into a cavity forming Ps. In reflective films Ps is formed only on the surface while in black films Ps is formed the whole volume. Applying the Tao-Eldrup model one can calculate that the mean size of nano-cavities is approximately 5 Å.

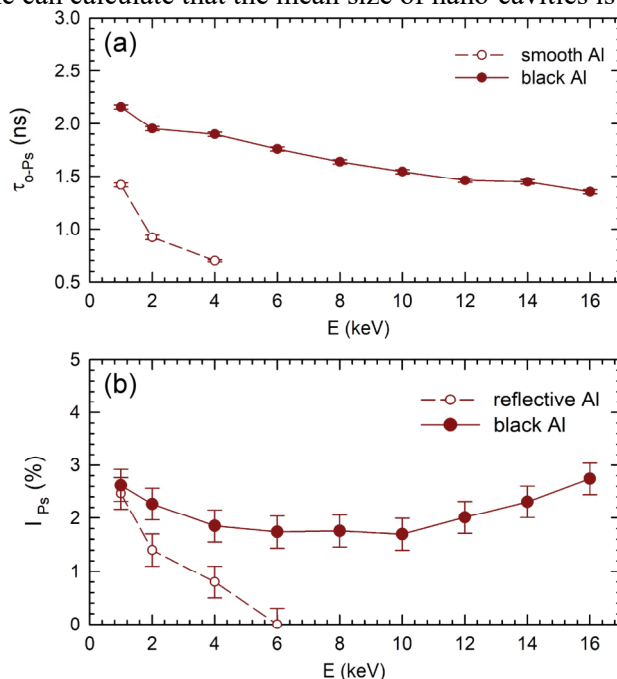


Figure 1 o-Ps lifetime (a) and intensity (b) for reflective and black Al film with thickness 20 μm .

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Manifestation of Vacancy-As complexes in As doped GeSn epilayers

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Epitaxial GeSn films doped with Arsenic are suitable for source-drain (S/D) stressors of n-FETs to obtain a sufficient conductivity of the source and the drain area. S/D stressors boost the carrier mobility to improve transistor performance [1]. Moreover, As is a possible candidate in order to overcome issues in forming n-type Ultra-shallow junctions (USJs) on Ge [2]. During the process of active doping with As, vacancies are formed in the GeSn:As epilayers. However, vacancy complex ($V_x\text{-As}_y$) level increases resistivity of the GeSn:As epilayers by passivating dopants along with a reduction of the lattice strain induced by As atoms.

Positron annihilation spectroscopy (PAS) is well suited to investigate vacancy complexes in narrow band gap semiconductors. PAS technique in Doppler and Coincidence Doppler mode was applied on GeSn epitaxial layers (thicknesses ~ 70 nm), grown by chemical vapor deposition with different mass flow ratio ($\text{AsH}_3/\text{GeH}_4$), high active As concentrations ($\sim 10^{19} \text{ cm}^{-3}$), and similar Sn concentrations (6-6.7%). Positron traps are identified as mono-vacancy complexes. Larger mono-vacancy complexes ($V\text{-As}_x$) are formed with the increase of the As concentration. ($V\text{-As}_x$) complexes increase the dopant deactivation of the sample epilayers. The mass flow ratio shows a significant impact on the defect distribution in GeSn layer.

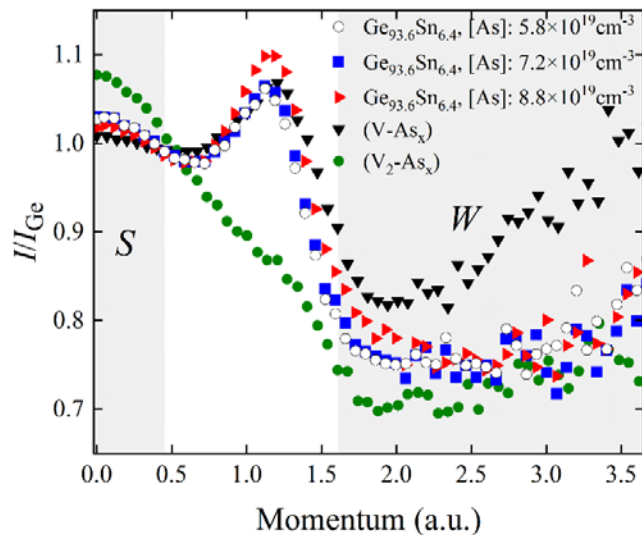


Figure 1 Annihilation intensity ratio for three different samples with CDOBS. Data were compared with two previous studies. ($V\text{-As}_x$) was studied from ref [3], whereas, ($V_2\text{-As}_x$) was analyzed from ref [4].

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The influence of trace elements on the formation of quenched-in vacancies in Al-alloys

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Strengthening of Al-Cu alloys is mainly controlled by the formation of copper-rich precipitates, so called Guinier-Preston zones (GPZ). Their size, distribution, and crystal structure plays a key role in defining the mechanical properties of these alloys (see Fig.1 right). It has been reported that the addition of trace elements such as In or Sn influences the formation of GPZs and, thus, the strength of the alloys by a strong binding of trace element atoms to quenched-in vacancies [1]. The presence of In or Sn influences the diffusion of Cu atoms and, thus, the formation of GPZs. Positron annihilation spectroscopy is used to study the interaction of trace element atoms with quenched-in vacancies. In pure Al-1.7 at% Cu alloys GPZs containing Cu monovacancies are formed after quenching into ice water. The GPZs evolve into the Θ' -phase during further heating. We performed theoretical calculations of positron lifetimes and found them to agree well with experimentally obtained values. While some trace elements (In or Sn) form thermally stable complexes and, thus, freeze out the mobility of vacancies, other trace elements such as Pb, Bi and Sb display nearly no effect in Al-Cu alloys: the average positron lifetime is very similar to that of the pure Al-Cu, indicating a small binding energy of vacancies to these elements. However, when binary alloys were quenched to -110°C (163K), they showed a high average positron lifetime, and thus a high concentration of vacancies (see Fig. 1), corroborating that the binding energy of vacancies to trace elements like Pb, Bi, or Sb is small.

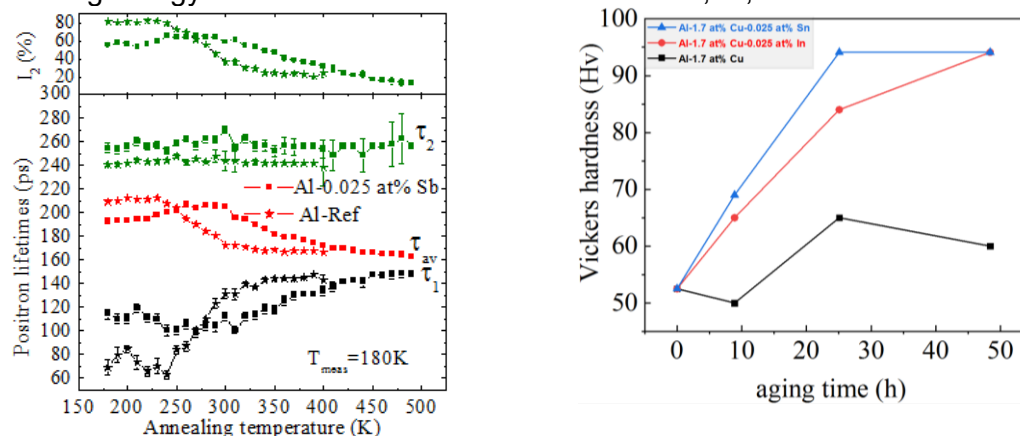


Figure 1 Al reference and Al-0.025 at% Sb after rapid quenching from 620 to -110°C (163K): positron lifetime as a function of isochronal annealing temperature (left). The measurement is performed at 180 K. Vickers hardness of Al-1.7 at.% Cu with and without 250 ppm In or Sn aged at 150°C for different times [1] (right).

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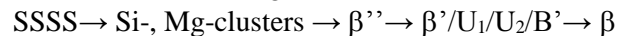
Artificial Aging of a Commercial Light Weight Alloy Studied by In-situ Positron Beam Doppler Broadening Spectroscopy

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Age-hardenable Al alloys with their main solutes being Mg and Si are widely used in automotive industry or for architectural and structural applications due to their low weight, high hardness and good corrosion resistance. These alloys obtain their maximum hardness by prolonged storage at elevated temperatures, a process referred to as artificial aging. During this heat treatment, precipitates grow within the Al matrix, which serve to harden the alloy by hindering dislocation movement. Although artificial aging is widely applied industrially the details of the precipitation sequence and especially the very early clustering stages are still under discussion; a rough model which is generally agreed on is the following [1]:



Here, SSSS refers to the supersaturated solid solution, β'' is a coherent phase, which is predominant in the peak-hardened microstructure, $\beta'/\text{U}_1/\text{U}_2/\text{B}'$ are semi-coherent phases and the equilibrium phase β is incoherent to the Al matrix. Especially initial clustering stages prior to the peak-hardened microstructure are of great interest to tailor the hardening response of the material. However, initial clustering takes place on short timescales and often only few atoms are involved which makes these precursor phases very difficult to investigate experimentally.

A unique opportunity to access these early clusters is the use of the positron beam of the NEPOMUC facility at FRMII. The high intensity of the beam enables Doppler broadening spectra acquisition at very short timescales, additionally the sample can be heated. This specifications made it possible to record the Doppler broadening S-parameter in-situ during artificial aging at two distinct temperatures, 180° C and 210° C.

The behavior of the S-parameter shows similar characteristics for the two applied aging temperatures, except for a temporal shift to longer aging times in the case of 180° C. Additional conclusions could be drawn from the comparison of this in-situ Doppler broadening data with ex-situ positron lifetime measurements and in-situ dilatometry [2]. Here, it has to be noted that the compared aging states for ex-situ and in-situ positron measurements are the exact same but the temperature of the sample during the measurements are different (ex-situ: -70° C, in-situ: 180° C/210° C). This affects whether positrons are captured (-70° C) or not captured (180° C/ 210° C) by shallow traps which appear in the alloy in the form of early clusters and small coherent precipitates [3].

In addition to the measurements during artificial aging at 210° C, the S-parameter was also recorded in-situ for the subsequent solution heat treatment of the very same sample. Here, with increasing temperature we could observe the dissolution of precipitates and the formation of vacancies.

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Effect of trace elements and quenched-in vacancies on precipitation hardening in Al-1.7at%Cu alloy

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Al-Cu alloy is a common precipitate hardenable alloy which is used in many industrial applications such as fuselage in aviation and automobile [1]. Microalloying is a typical method to control precipitation behavior as well as mechanical properties of Al-Cu alloy [2]. Here we study the influence of trace elements In, Sn, Sb, Bi and Pb (100 ppm) and their interaction with quenched-in vacancies on the precipitation decomposition in Al-1.7at% Cu alloy (5N5 base Aluminum) during ageing by PAS techniques. In and Sn are bound to quenched-in vacancies at RT and up to 150 °C and hence prevent copper atoms from diffusion which in turn change the precipitation sequence. On contrary, Sb, Pb, and Bi, which have theoretically high binding energies to the quenched-in vacancies [3], show no interaction with the vacancies. Free vacancies as well as In and Sn atoms accelerate precipitation kinetics i.e. nucleation of θ' phase which is the reason of the peak hardness.

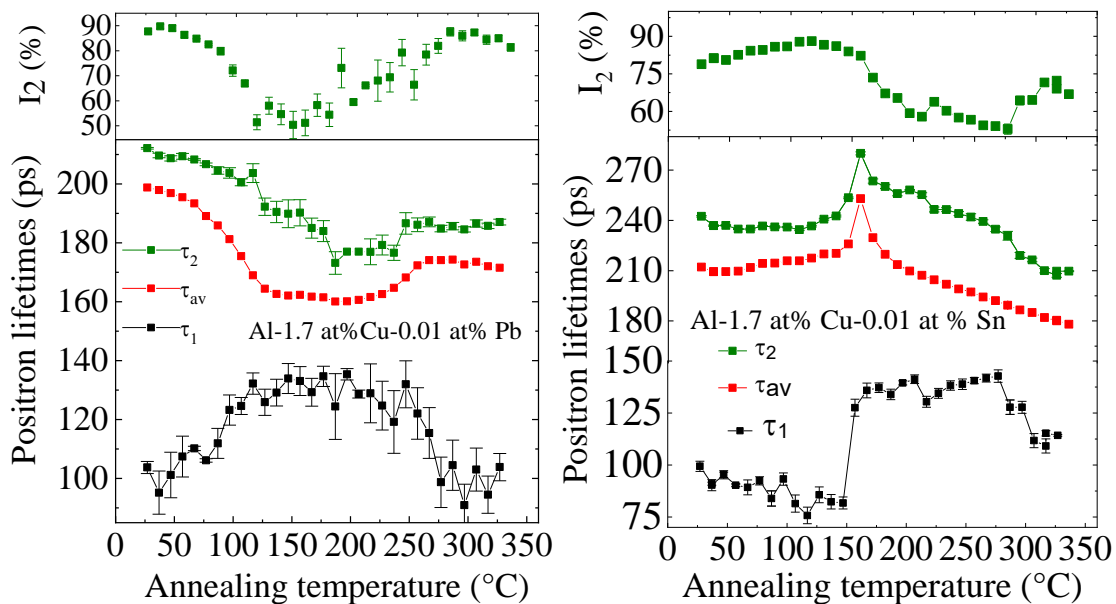


Figure 1 Positron annihilation lifetime measurement of quenched Al-1.7 at.% Cu with 100 ppm Pb and Sn as a function of isochronal annealing. Both alloys quenched at 520°C to ice water.

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Vacancies-solutes interactions and their role in the formation of oxide nanoparticles in ODS steels

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Oxide-dispersion strengthened (ODS) steels are good candidates for the structural materials of blanket/first-wall in fusion reactors as well as fuel cladding in advanced fission fast reactors. In these environments, ODS steels are submitted to hard conditions: high temperatures (500°C-1000°C) and high level of damage (200dpa). Their good properties are induced by the fine dispersion of low size oxide nanoparticles (Y, Ti, O). However, this nanoparticle distribution is often not controlled. It has been shown by theoretical models that the presence of vacancy during mechanical loading has to be considered as a key point for the control of the formation mechanism of these oxide particles and their composition.

In our experimental work, we have performed implantations with Y, Ti, O ions with several energies into high purity Fe samples (99,99%) in order to simulate the mechanical alloying step used for ODS steel fabrication. A slow positron beam coupled to a Doppler broadening spectrometer (SPBDB) was used to characterize the vacancy defects and vacancy-solute interactions. The solute depth profiles were measured using secondary ion mass spectrometry (SIMS).

The effect of annealing temperature on the defects and solute profiles was studied up to 550°C. The results show several evolution stages such as the disappearance of vacancy defects and precipitation of solutes. SIMS analysis showed that titanium and yttrium do not migrate during annealing experiments while oxygen shows a complex behavior of migration and trapping that depends on the material microstructure. SPBDB results show that solute implantations produce vacancy clusters, dislocations and vacancy-solute complexes. Their proportions evolve as a function of depth and nature of the implantations. Vacancy clusters and dislocations are detected deeper than the implantation peak with a higher fraction for the dislocations indicating that the defects were able to migrate during implantations. Vacancy-solute complexes are detected in the ion stopping zone and it is in a good agreement with the theoretical binding energy calculations. The nature and the distribution of the defects evolve according to the annealing temperature. Vacancy clusters disappear between room temperature and 300°C while the dislocations are eliminated from 400°C. Oxide phases are detected for annealing at 500 and 550°C due to the oxygen contamination during these annealing.

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Doppler broadening experiments (and calculations) in β -Ga₂O₃: vacancy defects, signal anisotropy, or both?

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We have applied slow positron beams and fast positron spectrometers with the intention to study vacancy-type defects in a wide variety of β -Ga₂O₃ materials: unintentionally doped and Si and Sn doped hetero- and homo-epitaxial thin films grown by metal-organic chemical vapor deposition (MOCVD) and halide vapor phase epitaxy (HVPE), as well as Mg, Fe and Sn doped bulk crystals grown by the Czochralski (CZ) and edge film-fed growth (EFG) methods. The data can usually be interpreted as the presence of varying concentrations of Ga vacancy related defects in some of the samples [1]. However, the colossal anisotropy of the positron annihilation signals makes quantitative interpretations cumbersome, as the magnitude of the anisotropy is comparable to the changes produced by annihilation at vacancy defects (compared to the annihilations in the “perfect” lattice) [2]. We report on a detailed experimental and theoretical investigation of the positron annihilation signals in β -Ga₂O₃ and provide an approach for identifying different kinds of vacancy defects based on the signal anisotropy. Interestingly, it appears that bulk-like positron signals might not be observed in any of the studied β -Ga₂O₃ samples.

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Positron Parameters for Atypical Samples (Rocks & Powdered Catalysts)

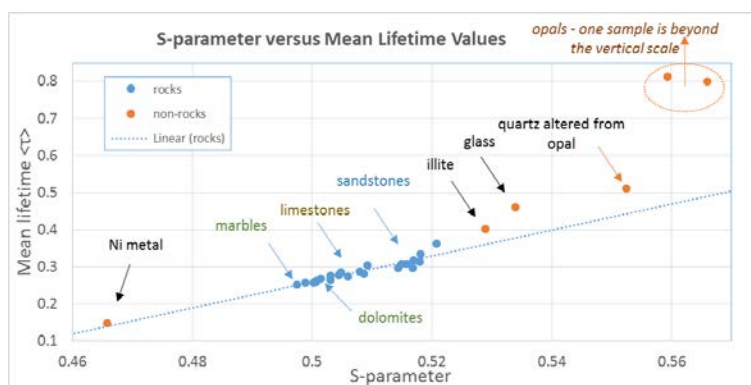
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Rocks, minerals and scarce amounts of powdered catalysts, not considered “typical” PAS materials were included in our studies. This work was done to find an appropriate method to characterize atypical materials in a unique way by proper set of parameters in a well-defined environment. The PAS analysis results were compared with other supplementary techniques including XRF, EDX, SEM, RGAS and BET analysis to understand the results better.

Although rocks are heterogeneous mineral aggregates, some PAS values were distinctly different for dry sandstones, limestone and dolomites. The mean lifetime and Doppler curve shape depended on rocks' conditions: dry, in brine or water; or state: solid or a powder. The PAS of rocks heated up to 200⁰ C revealed that the conventional S versus W-parameter ranges need to be modified to include the intermediate momentum range which was called SW-parameter. This was explained by a presence of different character of bonds, ionic and covalent, rather than metallic for which the division into S and W was defined to separate annihilation events due to free conducting electrons, or tightly bound core electrons. In summary, every rock/condition can be characterized uniquely by a unique set of mean lifetime and extended DBS values [1].



Additionally, opals in different stage of diagenesis and crystallization [2], and pure metals were examined. Fig.1 shows the relationship of S-parameter versus mean lifetime values. Different rock types are grouped tightly along the diagonal. The deviation of linearity is attributed to the intensity of Ps formation in some non-rocks.

Figure 1 S-parameter versus Mean Lifetime Values for Rocks versus non-Rocks

In contrast to rocks, catalyst zeolite powders represent another class of porous minerals. The obstacle that we encountered came from the fact that the samples were of low density and mass, usually less than 0.1 g, obtained from batches of fresh or processed through chemical reactors. We had to build special well-characterized sample holders to encapsulate the powder in thin Kapton film to prevent the potential contamination of the radioactive source and to optimize the geometry for enhancing positron annihilation event with the catalyst. We also used a sophisticated data analysis program for positron range analysis, LYS-1 [3], to determine the fraction of positron annihilating in the powder as compared to the source, Kapton envelope and backing [4]. When we used a well-controlled environment, and took into account matrix effects, the preliminary results of catalysts' PAS analysis became quite promising.

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Controlling the network properties of polymer matrixes for improvement of amperometric enzyme biosensors: Contribution of positron annihilation

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The development of new approaches for monitoring xenoestrogens as the most dangerous pollutants of wastewater is a topical problem to improve human life first of all. To do that, the most promising in analytical biotechnology seems to be amperometric biosensors – bioanalytical devices that combine the best features of bioelements (selectivity) and physical transducers (high sensitivity and accuracy). Establishment of the most suitable polymer matrixes and nanocarriers for immobilization of enzymes and construction of improved amperometric biosensors of the ‘third generation’ on the base of the created biorecognition films is a challenge and needs a lot of efforts. In the present study the organic (conductive polymers, photopolymers and others) and organic-inorganic hybrid (ureasil-composite, Nafion-composite and others) polymer matrixes with micro/nanoparticles (graphenes, nanoparticles of noble metals), oxide nanoparticles were used for immobilization of microbial laccase and construction of new prototypes of amperometric biosensors for potable water analysis with improved operational parameters (sensitivity, selectivity, stability, and reproducibility).

The knowledge of the properties of the microstructure of such polymer materials is important in terms of optimizing the regulated properties of the amperometric biosensors. A swelling test provides information about a crosslink density and flexibility of polymer network and is commonly used to characterize the structure of a cross-linked polymer. At the same time, positron annihilation lifetime spectroscopy (PALS) is known as a progressive method for microstructural analysis of macromolecular structures. Combination of these both methods allowed to get information about network properties of the polymer matrixes and the results obtained were further compared with sensitivity of bioelectrodes constructed using the polymer matrixes [1-4]. A role of free-volume and crosslink density in the host polymer matrixes used for improvement of operational parameters of laccase-based amperometric biosensors was established. Finally, it is found that the coefficients for the thermal expansion of free-volume holes α_{F1} , α_{F2} below and above T_g as well as their difference ($\alpha_{F2} - \alpha_{F1}$) obtained with help of PALS could be used as controlling parameters of polymer matrixes for improvement of functionality of amperometric enzyme biosensors constructed based on the polymer matrixes.

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Studies of alive normal and cancer cell lines and tissues in vitro with Positron Annihilation Lifetime Spectroscopy

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Positron Annihilation Lifetime Spectroscopy (PALS) allows examining structure of materials at nano and sub-nanometer level. It is mostly used for studies of inorganic materials, however it can be used for studies and imaging of the cell morphology as proposed in patent [1]. Cancer cells are characterized by an altered macro structure and activity in comparison to normal cells, thus the main aim of this studies is to compare if these differences can be detected on sub-nanometer level and therefore allows to distinguish between normal and cancer cells with application of PALS technique.

There exist few results, e.g. by group of Y. C. Jean [2-3] and J-PET [4-5] showing that morphology of cells is correlated with the PALS parameters. Preliminary studies shown significant differences in o-Ps lifetime between tumor (cardiac myxoma) and normal (lipid mediastinal) tissue and freeze-dried melanoma (cancer) and melanocytes (normal) cell lines.

Results of the first experiment with alive melanocytes and melanoma cell culture in vitro will be presented. PALS, viability and transcriptomic studies were performed on normal and cancer cells cultures, before and after measurement conducted in condition close to ones in human body (eg. in 37 C deg.). As a result, it was proved that PALS can be successfully used for studies of living organisms, their dynamics and its relation to the cells morphology. Second part of conducted studies were measurement of cells in presence of known antioxidants such as ascorbic acid and epigallocatechin gallate (EGCG) to check if changes of reactive oxygen species (ROS) level – free radicals present in higher concentration in cancer cells than normal ones, due to cell activity can be detected by PALS.

Results of studies with human tissue will also be presented. Research were conducted on two models: cardiac myxoma (benign hart tumour) with adipose mediastinal tissue as a control and colorectal cancer with normal colon (large intestine) tissue. All these studies shown significant differences in o-Ps lifetime between normal and cancer cells.

This result opens perspective for simultaneous determination of early and advanced stages of carcinogenesis by observing changes in biomechanical parameters between normal and tumour cells and standard PET examination. Such simultaneous PET imaging and PALS investigations can be performed with the Jagiellonian Positron Emission Tomograph (J-PET) [6-9] which is a multi-purpose detector used for investigations with positronium atoms in life-sciences as well as for development of medical diagnostics. J-PET is capable of imaging of properties of positronium produced inside the human body [1, 8].

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Progress in the study of energy tunable Ps beams employing the Ps⁻ photodetachment technique

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In 2012, an energy-tunable Ps beam employing the Ps⁻ photodetachment technique was developed [1]. An efficient method to produce Ps⁻ ions using a Na-coated tungsten surface enabled this development [2]. The beam provided an energy range that extended to a few keV, which was a hitherto unrealized range and complementary to that of the beams produced using the charge-exchange reaction with gas molecules [3]. This system has enabled the observation of the shape resonance of Ps⁻ [4]. However, further applications were limited because Ps⁻ ions were emitted from the thick tungsten target in reflection geometry and the trajectory of the Ps beam overlapped with the incident positrons.

In order to obtain Ps beams available for many applications, we have investigated the Ps⁻ production using a thin tungsten film in transmission geometry. When low-energy positrons impinge on a tungsten film, they lose their energy until they are thermalized in the bulk and then diffuse back to the surface. We found that the thermalized positrons which diffuse to the opposite surface also contribute to the Ps⁻ production if the film thickness is on the order of 100 nm.

Recently, we have completed a new Ps beam apparatus using this geometry at Tokyo University of Science [5]. Slow positrons from a ²²Na source capsule and a solid Ne moderator are pulsed using a buffer gas positron trap (Surko trap) and then focused onto a tungsten film of 100 nm thickness with a magnetic lens. A fraction of the positrons are emitted as Ps⁻ from the opposite surface coated with Na. The Ps⁻ ions are accelerated and photodetached by a pulsed laser light. The Ps beam energy range is 0.2 – 3.3 keV. The size of the Ps beam spot observed using a MCP located 419 mm downstream from the photodetachment point is 9 mm. It can be reduced further using a narrow aperture.

Using this beam, new experiments have started. In this talk, the details of the beam will be presented and the experiments will be discussed.

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Positronium Formation at Metal, Semiconductor and Graphene Surfaces

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Positrons implanted into the subsurface region of a material diffuse back to the surface and are emitted as positronium by picking up surface electrons when the positronium work function is negative. When positronium is formed, positrons select electrons at the vacuum side of the surface, where the screening effect of the Coulomb potential is adequately reduced. Because of the energy conservation law, the electrons occupied below the Fermi level to the positronium work function contribute to the positronium formation. The angular distribution of emitted positronium reflects the electron momenta, i. e., the band dispersions. Using the spin polarized positrons, electron spins can also be detected. For these reasons, ‘Positronium spectroscopy’ may be a potential tool to investigate the electronic structure of solid surface. In the photoemission measurement, electrons in ~nm depth are detected on average and hence it is not easy to specify which layers the electrons come from. One advantage of positronium spectroscopy is its top-surface sensitivity. To establish the positronium spectroscopy, positronium formation process needs to be revealed in detail.

So far, the positronium formation process has been studied mainly for metal surfaces. However, the theoretical understanding is still not sufficient. The investigation of semiconductor surfaces and furthermore single-layer materials such as graphene is remained nearly untouched. Application of spin-polarized positronium spectroscopy is not extensively progressing. In this paper, we will report (i) theoretical interpretation of positronium energy spectrum of metal surface [1], (ii) positronium formation at Si, SiC and graphene/SiC surfaces [2] and (iii) spin-polarized positronium annihilation at ferromagnetic surfaces [3].

For (i), we attempted to reproduce the positronium energy spectra at Al(111), Ni(111), Pt(111) and W(100) surfaces based on the Ishii’s theory and first principles calculation. We found that the dissociation of once generated positronium due to the interaction with remaining hole needs to be considered to reproduce the experimental spectra. For (ii), we found that there are two types of positronium distinguished from their kinetic energies at Si and SiC surfaces. For (iii), we found the spin-polarized electrons in graphene grown on Co(0001), Ni(111), Fe(110) and Co₂FeGaGe(001) surfaces .

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Damage induced by irradiation in W and deuterium trapping in vacancy defects probed by slow positrons

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Tungsten has been chosen to cover the divertor and is envisaged for first wall material in fusion power reactors because of its high melting point, good thermal conductivity, low thermal expansion, high strength at high temperatures and high sputtering threshold energy. In such systems, tungsten will be submitted to neutron irradiation, high Helium and Hydrogen (deuterium and tritium: the fuel mixture) fluxes, and high heat fluxes up to $10 \text{ MW}\cdot\text{m}^{-2}$ in stationary and up to $20 \text{ MW}\cdot\text{m}^{-2}$ in transient operation and will have to sustain a temperature up to 1780 K. Such severe operating conditions could have a high impact on the macroscopic properties of the material, such as embrittlement and swelling. Furthermore it is of most importance to foresee what will be the quantity of tritium retained in the wall of the tokamak.

In order to study and understand the evolution of the microstructure of tungsten under conditions similar to those expected in future fusion reactors such as ITER and DEMO, well-prepared high purity tungsten samples were irradiated with W ions at 1.2 MeV and 20 MeV for damage doses between 0.01 and 0.4 dpa and for temperature of 773K. Vacancy type damage induced close to the surface (first 700 nm) was probed using Positron annihilation spectroscopy. Both Doppler and lifetime spectrometries were performed using slow positron beams: the CEMHTI-Orleans slow positron beam for Doppler measurements and the PLEPS set-up for Lifetime spectroscopy at the NEPOMUC facility at the MLZ in Garching. The positron results are compared with Transmission Electron Microscopy (TEM) observations for some conditions. In this paper the effect of the damage dose on the distribution of vacancy type defects and the evolution of the positron annihilation characteristics after deuterium exposure will be discussed.

Acknowledgements:

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Effect of Defect Production on Photoluminescence & Positron Trapping in He ion Implanted Methylammonium Lead Tri-Iodide Perovskite Layers

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Hybrid inorganic-organic halide perovskites attract much attention for their application in optoelectronic devices. However, the performance in domain such as photovoltaics still strongly depends on the quality of the active layers and their capacity to stand device operation without irreversible damage. Applying a bias in dark in CH₃NH₃PbI₃ (MAPbI₃) based solar cells results in ion migration [1]. This questions the generation and role of defects under bias and light illumination [2,3] on photovoltaic performance.

In this work, Helium ion implantation is used as a tool for the introduction of point defects in a controlled way in polycrystalline MAPI layers spin coated on glass/ITO/PEDOTT:PSS. The created point defects may introduce energy levels and modify electronic and light emitting properties of the material. The defect production has a strong effect on photoluminescence (PL), time-resolved photoluminescence (TRPL) and PAS spectra. The results illustrate how the optical and positron behavior depend on the layer history before and after He ion implantation.

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Effect of rhenium on microscopic defects induced by He-ions irradiation in tungsten-based alloys

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In order to study the effect of transmutation element (Re) on the micro-defects of tungsten (W) in plasma environment, positron annihilation spectroscopy [1,2,3] was utilized to characterize the distribution of vacancy-type defects in W and W5Re alloys irradiated by He-ions beams with different energies and fluences (16 keV@ 5.8×10^{20} ions m^{-2} for W-1 or W5Re-1, 70 keV@ 1×10^{21} ions m^{-2} for W-2 or W5Re-2, 200 keV@ 2.4×10^{21} ions m^{-2} for W-3 or W5Re-3, respectively). It was found that when the irradiation dose was less than 10^{21} ions cm^{-2} , the distribution of vacancy-type defects in W5Re alloys was almost consistent with that in tungsten. When the dose increases, the effect of Re on the electron density distribution at the defect site becomes obvious. Positron annihilation lifetime results show that the defect concentration of the W sample added with 5 wt.%Re will be significantly higher than that of pure tungsten, while the longer lifetime value decreases significantly. Re will restrain the growth of vacancy-type defects to a certain extent, thus affecting the conformity between interstitial He atoms and vacancies, which will result in the strong display of helium information around the defect sites.

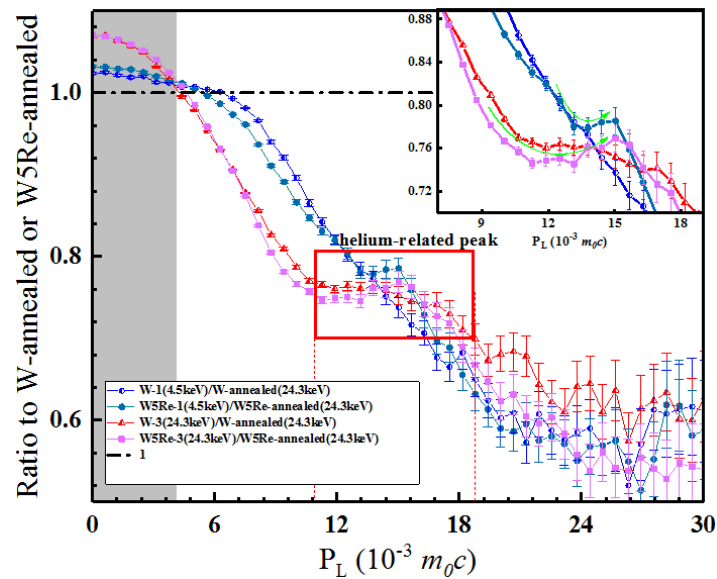


Figure 1 CDB curves for W-1/W-annealed and W5Re-1/W5Re-annealed with a slow positron beam of 4.5 keV, and for W-3/W-annealed and W5Re-3/W5 with a slow positron beam of 24.3 keV.

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Positron annihilation studies of reactor pressure vessel steels treated by irradiation and hydrogen ion implantation

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Long term operation of nuclear reactors is one of the most discussed challenges in nuclear power engineering. The radiation degradation of nuclear materials limits the operational lifetime of all nuclear installations or at least decreases its safety margin. This paper is focused on experimental simulation and evaluation of materials via hydrogen ion implantation and comparison to our previous results obtained from neutron irradiated samples. In our case, German reactor pressure vessel steels, originally from CARINA/CARISMA program, were studied by positron annihilation lifetime spectroscopy and pulsed low energy positron system with the aim to study microstructural changes in RPV steels after high level of irradiation [1]. Unique specimens were irradiated by neutrons in German experimental reactor VAK (Versuchsatomkraftwerk Kahl) in the 1980s and these results were compared to results from high level of hydrogen nuclei implantation. Defects with the size of about 1-2 vacancies with relatively small contribution (with intensity on the level of 20-40 %) were observed in all “as-received” steels. The increase in the size of the induced defects due to neutron damage was observed in the irradiated specimens resulting in 2-3 vacancies. On the other hand, the size and intensity of defects reached extremely high values due to displacement damage caused due to implantation of hydrogen ions in very narrow damaged region. This fact can limit operation of new fission or fusion nuclear facilities [2].

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Effect of carbon on the evolution of early stage radiation defects in equi-atomic CoCrFeMnNi high-entropy alloys

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Due to the excellent fracture toughness, irradiation and corrosion tolerance, High-Entropy alloys (HEAs), or concentrated multicomponent alloys have been drawing much attention and have the potential to be developed as new structural materials in extreme condition. Recent research showed that carbon addition improved the strength and ductility simultaneously in face center cubic (fcc) HEAs [1, 2].

In order to understand the carbon effect on microstructure evolution in early stage irradiation damaged HEAs, 150 keV hydrogen ions were implanted in C-containing equi-atomic CoCrFeMnNi high-entropy alloys at room temperature. The irradiation fluence were ranged from 2.5×10^{14} up to 2.5×10^{17} ions/cm² and the damage dose were estimated between 0.001 dpa and 1dpa by using SRIM calculation. Doppler broadening spectroscopy based on slow positron beam [3] was utilized to characterize the radiation defects and the microstructure evolution in as-irradiated samples. The results indicate that mono-vacancies generated in samples during early stage irradiation process, and the irradiation induced point defects migrated and accumulated to vacancy clusters as the irradiation dose increasing. The addition of carbon interstitials interact with irradiation vacancies to form C-vacancy complexes, which suppress the migration and coalesce of point defects and furthermore enhanced the irradiation tolerance of CoCrFeMnNi high entropy alloys.

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In Situ Ion Implanter to Study Vacancy-Impurity Interactions

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We have constructed apparatus which allows ion implantation from a gas source, at energies to ~30keV over a temperature range of ~20K to 900K, alternating with positron characterization by Doppler broadening, with positron energies to ~30keV.

Data will be shown comparing in-situ implantation into silicon vs. an ex-situ low-energy ion implanter for system calibration. Preliminary experiments to study defect mobility by implantation at 100K and subsequent isothermal annealing will be described.

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Defect and ion distribution studies in ion-implanted silicon

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Ion implantation is one of the most important doping technique in planar technology. During irradiation a lots of defects are created which affect material properties. Positron annihilation techniques allow one to study type and concentrations of the open-volume defects i.e vacancies. The ion projectile range and vacancies depth profiles can be calculated using widely available programs such as SRIM/TRIM. The produced defects mostly occupy the same area as the implanted ones. However, some experiments have shown a much complex damages distribution which is extended much beyond the projectile range.

In current studies the Doppler broadening of the annihilation radiation depth profiling technique was applied to investigate the effect of dose variations in pure silicon. Variable-energy positron beam studies in Ar, N and C ions irradiated silicon have been conducted. Si samples were irradiated with 25 keV ions with doses $2 \cdot 10^{14}$, $2 \cdot 10^{15}$ and $2 \cdot 10^{16}$ cm⁻². Ion distribution of C and N implanted samples was obtained using glow-discharge optical emission spectroscopy method. The variation of S parameters show a maximum corresponding to maximum damage calculated with TRIM, but defected zone for highest dose extend far beyond implanted ions indicating on long range effect. Also influence of ion dose on defect concentration was noted.

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Ion beam modification of crystalline materials for optoelectronic application

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Doping and dopant diffusion control in GaN is not only important for green to ultraviolet (UV) light-emitting diodes, lasers, and detecting devices but also for high-frequency, high-temperature, and high-power electronic devices. Ion beam implantation is very powerful, versatile and unique technique enabling creating of supersaturated layer and by changing the implantation parameters tuning the optical and electrical properties. It has been found that the ion-beam-induced processes in various crystallographic orientations influence the defect accumulation, which is closely connected to the optical and electric properties of the films. An attempt was made in this study to coax the optical properties of various crystallographic orientations to enhance the understanding about the interaction of implanted specie with the crystalline substrate. The various crystallographic orientations in semiconductors as ZnO, GaN exhibit different resistivity under the ion beam irradiation/implantation and study of various crystalline orientations is mandatory for the nano-structured semiconductor systems, as they exhibit several facets which are modified during ion beam implantation. It has been shown that ZnO exhibit strong dynamic annealing i.e., migration and interaction of ion-beam-generated defects during ion irradiation and much lower surface damage accumulation comparing to GaN. Structure, morphology, and optical properties of Gd, Er, Au, implanted GaN and ZnO, layers and bulk crystals were studied in a-, c- and m-plane using the distinct ion energies from 200 keV to 5 MeV. Dopant depth profiling was accomplished by Rutherford Back-Scattering spectrometry (RBS). Structural and optical changes during subsequent annealing were characterized by RBS, Raman spectroscopy, and photoluminescence measurements. Surface morphology was investigated by AFM and Scanning Electron Microscopy. Post-implantation annealing induced a structural reorganization of crystal structure in the buried layer depending on the introduced disorder level, i.e. depending on the ion implantation fluence and on crystallographic orientation. The defect density depth distribution was evaluated by RBS. The surface morphology and optical properties depend on particular crystallographic orientation.

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Microstructure and nanoscopic porosity in black Pd films

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Thermal evaporation of metals in carefully adjusted low pressure (~ 100 Pa) of N_2 gas enables deposition of peculiar porous structures known as black metals. Surface of black metals appears dark since light incident on the surface is completely absorbed in multiple reflections in fractal-like structure of percolated micro-cavities with a broad size distribution. Black metals can be used in electronic devices for optical sensing, camouflage and gas sensors. The physical mechanism leading to formation of black metals is not completely understood yet and parameters for their preparation were found empirically.

In the present work microstructure of black Pd films deposited on Si single crystal and glass substrates was studied. Black Pd films were compared with smooth films. Typical microstructure of black Pd film is shown in Fig. 1a. Positron lifetime spectra of black and smooth Pd film are compared in Fig. 1b. Positron lifetime spectrum of black Pd film contains a long-lived component originating from pick-off annihilation of o-Ps. In conventional metals Ps does not form because any bound state of positron and electron is quickly destroyed by the screening of conduction electrons. However, in porous metals containing micro-cavities a thermalized positron may pick an electron on inner surface and escape into a cavity forming Ps.

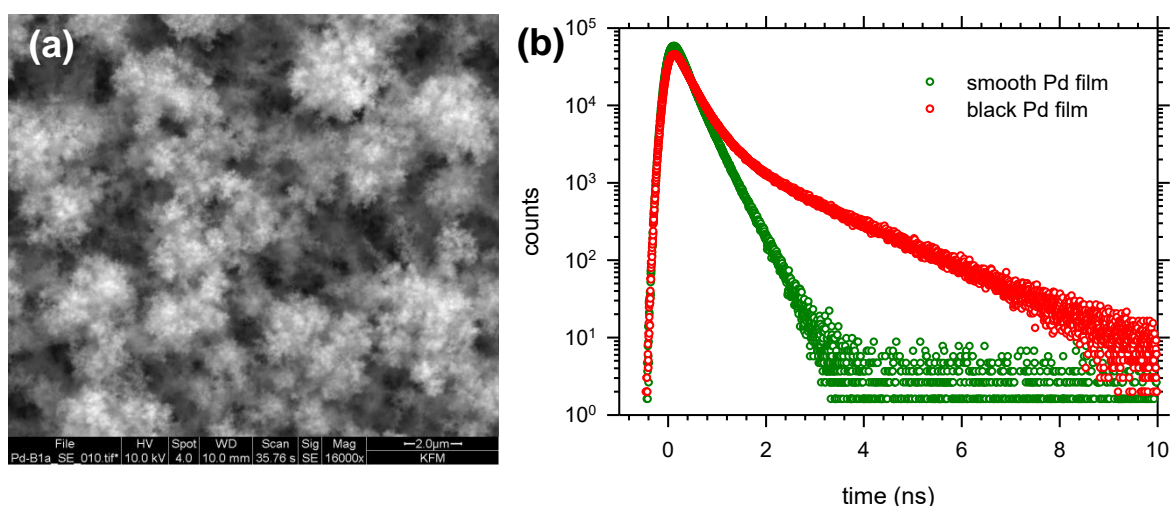


Figure 1 (a) Microstructure of black Pd film deposited on Si substrate, (b) comparison of positron lifetime spectra for smooth and black Pd film measured at positron energy of 8 keV.

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Positron annihilation at grain boundaries in lithiated and delithiated Li_xFePO_4 battery material

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The LiFePO_4 battery cathode material [1] is employed in various devices, including electric cars and bicycles, (mobile) home appliances, path/security lights, *etc.* This material possesses some advantages over frequently used LiCoO_2 -based materials, except slightly lower energy density. Nevertheless, LiFePO_4 materials can be further optimized and as a help in this process studying the structure and other properties of grain interfaces in cathodes made of small grains (powders) is necessary. The point is that Li ions are diffusing in and out of the grains – via the grain interfaces, which is an important aspect of the battery operation (discharging and charging).

The selected grain boundaries (GBs) in LiFePO_4 and FePO_4 were constructed by means of the coincidence site lattice geometrical concept [2] adapted to $(\text{Li})\text{FePO}_4$ orthorhombic crystal system. Initial atomic configurations/supercells containing up to 200 atoms were then relaxed using a pseudopotential electronic structure code based on the density functional theory considering the magnetism of the studied system. Positron characteristics such as lifetime and positron binding energy to GBs were determined using relaxed configurations. The bulk positron properties of LiFePO_4 and FePO_4 were calculated already earlier [3]. Structural and positron calculations show that studied grain boundaries exhibit free volumes where positrons can be trapped. The GBs in FePO_4 have longer lifetimes. The comparison with positron lifetime data for a powdered LiFePO_4 sample (grain size ~ 100 nm) [4] suggests that one lifetime component could originate from the GBs. This indicates that positron annihilation spectroscopy could in principle be used to study grain interfaces in Li_xFePO_4 system and probably also in other Li-ion battery cathode materials. Possible ways of Li diffusion at GBs in the studied material are also discussed.

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Measurement of annihilation lifetime for positron burst

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High intensity positron bursts, with a time spread of few nanoseconds or even picoseconds, can be produced thanks to the development of positron trapping and femtosecond laser-induced positron techniques. Huge number of gamma photons will be released at almost same time, when the positron burst annihilates in the target. Because of the overflow of detector, it is impossible to pick out the time information for each annihilating γ -ray using conventional time-measurement nuclear detection technology. In this study, the method of a multi-detector array composed of enough independent detector cells, with high efficiency and accuracy, is first put forward to detecting the positron burst lifetime.

The performance parameters of timing resolution and counting efficiency for a PALS measurement by this method were simulated and tested in experimental. We found that the detection efficiency mainly depends on single γ detection efficiency of the detector cell and the intensity of the positron burst, the higher the efficiency of detector cell or the intensity of positron burst is, the larger detection efficiency the detector array system has. While the time resolution mainly depends on the burst time width and time resolution of detector cells.

When the burst detection efficiency of a detector cell is high enough, it is very likely to detect one more γ rays during one positron burst, and signals pile-up will occur. Due to the relatively long response time of detectors, pile-up leads to picking out the time information of the first photon that hits the detector only, and the information of other photons will be lost. Results showed that the positron lifetime value measured will be less than the true one with high pile-up level. In this work, we have analyzed the pile-up reason from three aspects—theoretical calculation, simulation and experiment. According to the results, the lifetime can be measured precisely by setting the signals' amplitude an upper-threshold corresponding to the energy of 511 keV. And the valid burst detection efficiency will be maximum ($\sim 37\%$), when the detector is at the position where the average number of γ -ray detected in a burst is only one.

In future, we plan to arrange 2048 detector cells on a hemisphere as the array. In order to detect lifetime efficiently and accurately, we found that once the properties of the detector cell and the intensity of the positron burst are fixed, the position and the valid detecting efficiency are determined. For example, for $3\text{mm}\times 3\text{mm}\times 5\text{mm}$ LYSO and 5000 e^+ /burst with 33 Hz repetition frequency, the array radius is 54~85 mm and the typical counting rate can reach $2.5\times 10^4/\text{s}$.

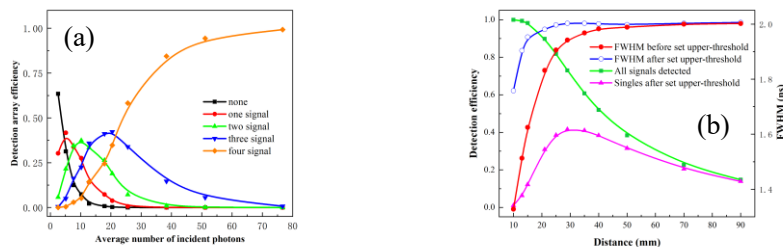


Figure (a) Detection array efficiency as a function of the average number of incident photons. **(b)** FWHM of 2ns width burst and detection efficiency as a function of the detector distance.

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Early stages of precipitation in mould-cast, cold-rolled and heat-treated aluminium alloy AA7075 with Sc,Zr-addition

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Precipitation reactions of the commercial Al–Zn–Mg–Cu(–Sc–Zr) alloy in the mould-cast, cold-rolled and heat-treated states were characterized by electron microscopy, X-ray diffraction, thermal analysis, microhardness testing and positron annihilation spectroscopy. The initial microhardness values of the alloys reflect the cold rolling. The distinct changes in microhardness curves as well as in heat flow of the alloys studied are mainly caused by the dissolution of the clusters and precipitation of the particles from the Al–Zn–Mg–Cu system. Easier diffusion of Zn, Mg and Cu atoms along dislocations is responsible for the precipitation of Zn,Mg,Cu-containing particles at the lower temperatures compared to the mould-cast alloys. The mould-cast and cold-rolled alloys contain solute clusters rich in Mg and Zn. Clusters formed in the heat-treated alloys during natural ageing have similar composition but in addition to Mg and Zn contain also Cu. The Cu-concentration increases with increasing period of natural ageing. The mould-cast state and state after natural ageing contain in addition to solute agglomerates also vacancy clusters formed by agglomeration of thermal vacancies. Addition of Sc and Zr results in higher hardness above ~ 270 °C due to strengthening by the Al₃(Sc,Zr) particles with good thermal stability. Sc and Zr have probably no influence on the development of solute clusters.

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Positron Annihilation Analysis for Zeolites/Silica Gel used in Catalysis

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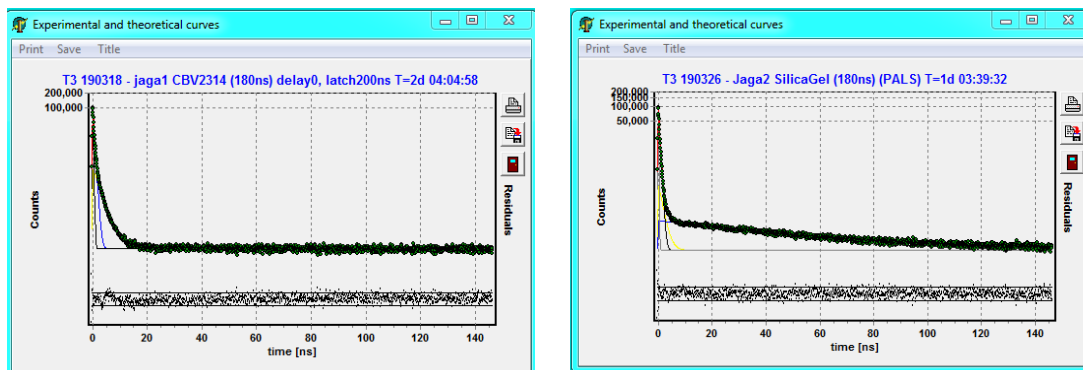
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Pelletized samples of zeolite (H-ZSM-5), silica gel and their mixture used in catalytic hydrocarbon processing, were investigated using Positron Annihilation Lifetime (PAL) and Coincidence Doppler Broadening (CDB). In the catalytic testing of methanol conversion to olefins it is necessary to dilute the H-ZSM-5 (catalyst) with inert silica to achieve more uniform changes in the material with time-on-stream, therefore the Zeolite/silica gel ratio equal 1: 3.054 for the mixture was used.

The PAL measurements were done in two different time regimes up to 150 ns to detect long lifetimes due to a Positronium (Ps) formation. The surface of the pelletized and non-pelletized (powder) samples were examined under an optical digital microscope to identify the effects of pelletizing, and the homogeneity of the mixture.

Fig. 1 PAL for H-ZSM-5 (left) & silica gel (right) by use of LT-9.2 program [1], extended time scale



Zeolites represent a class of porous minerals with uniform, regular and highly organized micro-structure. The PAL measurements showed 2.4 ns lifetime due to micro-pores: 0.3-0.4 nm diameter [2], with the intensity over 20% for pure zeolite, about half of this intensity for the mix, and none for the pure silica gel [Fig.1]. On the contrary, silica gel exhibited a 44 ns lifetime due to the meso-pores about 5 nm size [3], with intensity 24% for pure gel, 15% for the mix and none for the zeolite. These lifetimes can be used as unique fingerprints for characterizing zeolite versus silica gels and their mixtures.

The presence of a lifetime over 40 ns in silica gel in air suggest that the silica macro-pores are either closed or interconnected through the nano-channels that cannot be easily penetrated by oxygen, a prominent Ps quenching agent [4]. The CDB analysis of ratio curves indicates discrete structure of pure materials compared to less-defined structure of the mixture caused by a possible hybridization of the atomic states.

Novel positron annihilation spectroscopy results presented here will allow greater in-depth studies of the process of catalyst deterioration and deactivation and to understand how the process conditions of the chemical reactor affect the internal structure of the catalyst (e.g. via calcination, coking). Since both materials have distinct characteristics indicated by the PAL fingerprints due to different nature of internal structures, we hope to be able to study the process conditions that most greatly impact material ageing.

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Positron Spectroscopy of Defect Structure of Electron Beam Melted Titanium Ti-6Al-4V Alloy

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Nowadays additive manufacturing (AM) is being actively implemented in aerospace industry. Among the advantages of AM in metals are the possibility of creating unique product shapes, providing solid and lightweight (e.g. lattice) structures in a single manufacturing process and high quality of resulting materials. Additionally, electron beam manufacturing (EBM) technology today provides high rates of production and layer-to-layer component quality control. The use of additive manufacturing also allows creating a new generation of materials with unique set of properties. The same time few issues related to the EBM process in already well established AM materials like Ti and Ti-6Al-4V remain not clear [1-3]. Present paper reports results of the first studies into influence of manufacturing parameters on electron beam melted Ti-6Al-4V alloy defects structure by means of positron spectroscopy.

Positron spectroscopy (PS) methods are the most promising for controlling the small-size defect structure of additive manufacturing materials due to high sensitivity and the ability to determine the type of defects and concentration. Investigation of defects structures carries out by means of positron lifetime spectroscopy (PLS) and Coincidence Doppler broadening spectroscopy (CDBS) on semi-digital complex. The semi-digital complex has excellent technical characteristics using a positron source based on the ⁴⁴Ti isotope with the activity of 0.91 MBq (the resolution of the digital PLS module is 170 ± 7 ps, the energy resolution of the CDBS module is 1.06 ± 0.03 keV).

Positron lifetime spectra of samples with different beam current and speed function were fitted by three exponential components. The first one corresponds to the positron lifetime in the bulk of the material ($\tau_{Ti} = 147 \pm 1$ ps). Lifetime values of other two components τ_a and τ_b were referred to the annihilation of positrons trapped by dislocations ($\tau_{disl} = 165 \pm 3$ ps) and vacancy complex ($\tau_{nv} = 291 \pm 5$ ps) of titanium. The CDBS data also confirm the obtained data.

Depending on additive manufacturing parameters the density of dislocations varies in the range of $10^{13} \div 10^{14}$ m⁻², and the concentration of vacancy complexes - $10^{-3} \div 2$ ppm.

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Investigation of defect structure distribution in the multilayer nanoscale self-healing coatings based on Zr/Nb layers after proton irradiation

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Multilayer nanoscale coatings (MNC) with different crystal structures are considered as capable to self-healing after radiation damage due to the recombination of vacancies and interstitials. Most of the MNC studies are focused on the interrelation of the structural and strength characteristics [1, 2], but do not include investigation of defect structure. This work is focused on defects distribution study in MNC based on Zr/Nb layers (25/25 and 100/100 nm) after proton irradiation. Coatings with the total thickness of about 1-1.5 microns were irradiated by 900 keV protons using linear electrostatic particle accelerator with the ion current of 2 μ A during the time of 30 to 120 minutes. The influence of irradiation effect on the overall and, in particular defect structure was studied by X-ray diffraction analysis, discharge optical emission spectrometry and positron spectroscopy with the varied energy of positrons. It was shown, that defects concentration of MNC after proton irradiation does not increase and, in some cases shifts to the lower values. This effect can be explained by the presence of an incoherent two-layer interface, which traps the defects. This effect is more evident in the samples with the larger number of such interfaces (25/25 nm samples, see Figure 1).

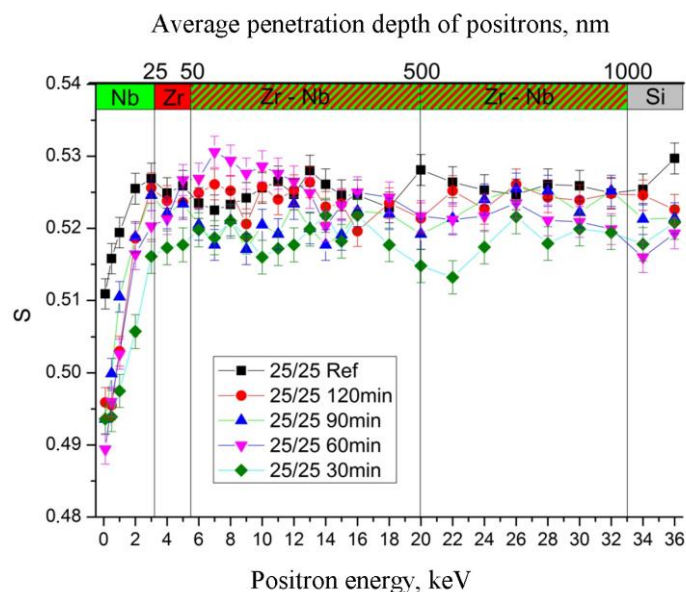


Figure 1 Dependence of S -parameter on positron energy in multilayered Zr/Nb coatings with the layers thickness of 25 nm and different proton irradiation time.

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Results of a supranational Round Robin Test to initiate an international standard for source-based PALS measurement

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The source-based positron annihilation lifetime spectroscopy (PALS) represents a very sensitive method to characterize open volumes / open volume defects on an atomic scale for a broad range of material classes such as metals, semiconductors, polymers and porous materials. Even though PALS has been established in the early 1960's, there exists up to now no standardization for measurement and analysis of the data. This leads to a significant lack of reliability in comparison to other methods used for the characterization of material properties.

In the aim to establish an international standard, several positron research groups in Europe conducted a Round Robin Test on a collection of nine well-known bulk materials (polymers, metals, semiconductors). All materials were shipped between the participants to ensure the best possible comparability. The kind of setup and the applied configurations have been documented. The correctness of the measurement procedures and software/algorithms used for data analysis has been tested.

A first draft of a standardized measurement procedure including a documentation form for the analysis were used to ensure that every participant does follow the process of the source-based PALS measurement.

Our suggested protocol is the first step towards an international norm for PALS measurements. A standardized documentation could help the positron community to reach a higher level of transparency, reproducibility and reliability and it would improve the comparability of PALS results obtained from different research groups. Furthermore, if the community agrees on a standard measurement procedure, it would increase the impact of any positron publication.

Our poster will give an overview of the results of the conducted round robin test. We will present the draft of a measurement and analysis template/form.

By this poster, we would like to provide a platform for all scientists in the field to discuss the idea of an international standard for PALS measurement. We invite all positron experts to discuss this idea to clarify, if it is possible and/or necessary to create such a norm.

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Absolute Differential Positronium-Formation Cross Sections From The Inert Atoms

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Absolute differential cross sections for ground-state positronium formation near zero degrees have been measured using the positronium beamline at UCL [1] from Ne, Ar, Kr and Xe targets [2], expanding and complementing previous work with Ar, He, H₂ and CO₂ [3]. The ratios of the differential to integral positronium formation cross-sections for each target will also be presented. These provide a measure of the degree of forward collimation of the positronium production process as a function of energy. Examples are shown in figure 1 for Ar. In addition, trends among targets have been observed consistent with the statistical description of inelastic processes [4] and will be discussed at the conference.

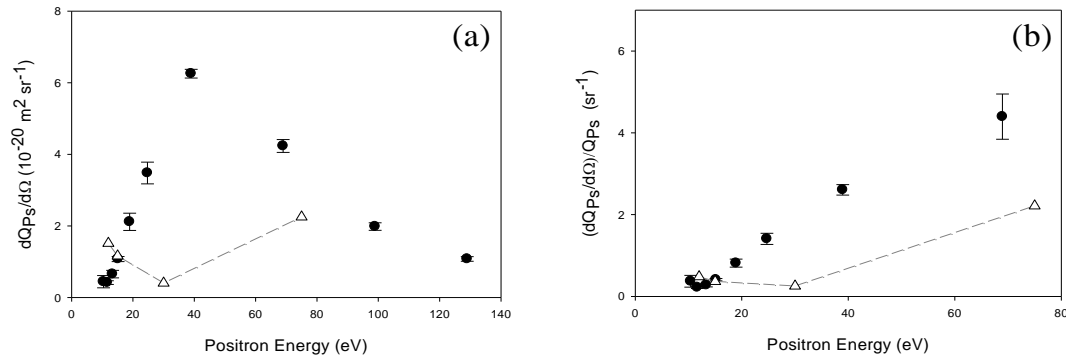


Figure 1. (a) Differential Ps formation cross section and (b) forward collimation for Ar near zero degrees [3]. Also shown are the truncated coupled-static calculation of McAlinden and Walters (triangles) [5] and a dashed line to guide the eye.

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PALS Avalanche – a new PAL spectra analysis software

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A novel concept for tomography of human body developed by Jagiellonian Positronium Emission Tomography (J-PET) [1-5] project provides the possibility to combine metabolic information collected by standard PET with structural information obtained from Positronium lifetime, in a concept of morphometric image [6]. Therefore, there was a need to develop compatible software with J-PET Framework [7], for fast online analysis during imaging.

PALS Avalanche [8] is a software developed on UNIX system and based on ROOT software, which allows to decompose Positronium Annihilation Lifetime (PAL) spectra collected by both digital and analog electronics. An unique iterative procedure and parameterization of intensities, implemented in PALS Avalanche, will be presented.

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The crucial defects induced in iron and stainless steel upon hydrogen embrittlement by positron annihilation spectroscopy

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Austenitic stainless steels are considered to be one of the most important structural materials for hydrogen energy systems. It is well-known that the Ni equivalent is strongly related to the hydrogen susceptibility and ANSI 316L with 12mass% Ni shows highly resistant to hydrogen embrittlement (HE). However, the hydrogen susceptibility is also dependent on a strain temperature and shows maximum around -70 °C. This phenomena is explained by the trade-off between hydrogen diffusion and stability of fcc-phase. Hydrogen stabilizes a formation of vacancies, so that it is very important to investigate their behavior in HE. In this study, austenitic stainless steels, ANSI 316L, strained at low temperatures were investigated by positron annihilation lifetime spectroscopy (PALS) and the crucial defects in HE were discussed. PALS is one of the most powerful methods to directly detect open-volume type defects in metals and enables us to obtain information on their size, chemical state and amount.

ANSI 316L sheets were exposed to 95 MPa of hydrogen gas at 300 °C for 72 h and the hydrogen concentration was estimated to be 90 ppm. The specimens were subject to tensile stress at temperatures from -150 °C to RT. ANSI 316L showed no hydrogen susceptibility at -150 °C and RT, while the fractured surface of the specimen straining at -70 °C showed the quasi-cleavage, indicating HE took place. The fractured sample strained at RT showed the formation of a lot of smaller vacancy clusters, indicating the agglomeration of the monovacancies. Hydrogen stabilized a formation of vacancies, so that the vacancies can homogeneously agglomerate to form small vacancy clusters because the stress-induced martensitic phase cannot form. On the other hand, larger vacancy clusters formed in the fractured sample strained at -70 °C. It is understood that the straining at -70 °C induced highly strained fields, such as at the boundary between the fcc and martensitic phases, where a lot of vacancy-hydrogen complexes locally formed and agglomerate to larger vacancy clusters. It is considered that they possibly become the embryos of the quasi-cleavage. The straining at -150 °C induced a lot of vacancy-hydrogen complexes and the formation of vacancy clusters could not be observed. Further, aging at RT lead to a formation of much larger vacancy clusters. It means that vacancies with a high density are locally formed, but they cannot diffuse and agglomerate at -150 °C. It is, therefore, concluded that the crucial defects upon HE in the austenitic phase are vacancy-hydrogen complexes with a high density induced by a strain localization. Further the results on the iron upon HE will be discussed.

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Construction of a spin-polarized positronium time-of-flight measurement apparatus

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Using spin-polarized positronium (Ps) annihilation spectroscopy, the electron spin polarization of top-surface layer can be determined because Ps is only formed at the vacuum side of the surface where the electron density is well-suppressed [1, 2]. So far, such measurements have been conducted without both energy and angular resolvabilities of Ps. If the energy-resolved and spin-polarized Ps annihilation spectroscopy is available, one can obtain the spin-polarized electron density of states associated with the top-surface layer of metals. The spin polarization at the Fermi level is very important to evaluate the spin transportation in devices in connection with the spin-Hall effect, Rashba effect and topological insulators. The spin-polarized Ps time-of-flight method (SP-PsTOF) will respond to such offers. We have been developing SP-PsTOF apparatus as shown in figure 1.

A spin-polarized positron beam generated from a ^{22}Na source (440 MBq) and a solid Kr moderator is transported to the sample by the electrostatic lenses avoiding depolarization. Beam energy can be controlled from 0.02 to 5.2 keV by applying a bias voltage to the sample. Time-of-flight of emitted Ps is determined by a time difference of a start and a stop signal. The start signal is triggered by secondary electrons detected by a Channeltron beside the sample. The stop signal is obtained from the ortho-Ps annihilation using NaI detectors with a lead slit. The sample is magnetized by an external electromagnet. By alternating the magnetic field direction, a difference Ps-TOF spectrum (SP-PsTOF spectrum) is obtained. Figure 2 shows a preliminary SP-PsTOF spectrum obtained for a Ni film. The negative polarization near the Fermi level, which is reproduced by a theoretical calculation, is measured. The further improvements of the apparatus are under the progress.

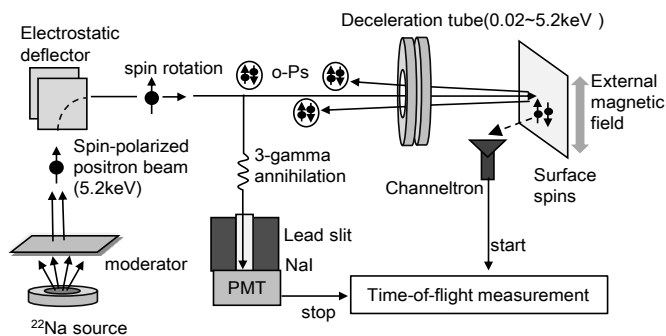


Figure 1 Schematics of spin-polarized positronium time-of-flight (SP-PsTOF) apparatus.

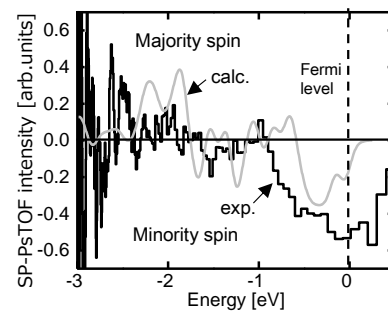


Figure 2 The test SP-PsTOF spectrum obtained for the nickel thin film.

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Improvement of positron lifetime measurement systems for the KUR slow positron beamline

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Energy-variable slow positron beams have been extensively used to investigate vacancy-type defects in thin-films and surface-modified layers (e.g., ion-implanted layers). Among major analytical methods of positron annihilation spectroscopy, positron lifetime annihilation spectroscopy (PALS) can give direct information on sizes of vacancy-type defects from lifetime values. Positron pulsing is one of the important methods to perform PALS measurements with slow positron beams. A slow positron beamline of Kyoto University research Reactor (KUR) has a pulsing system consisting of RF-driven chopper, prebuncher and buncher electrodes. This paper shows results of recent developments on the PALS measurements of the KUR slow positron beamline.

Performance of the pulsing system has been evaluated by electron beams in our previous study [1]. The best pulse width of 143 ps was obtained, indicating that the design of the pulsing system is appropriate. Numerical simulation of the pulsing system was also performed using the SIMION and GPT codes. It revealed the importance of uniform electric fields among pulsing electrodes. Even after these evaluation procedures, it has been difficult to obtain appropriate PALS results with our pulsing system. A series of experiments suggested that the PALS measurements using the KUR slow positron beamline is influenced by background radiation ($\sim 1 \mu\text{Sv/h}$ during 1 MW operation) caused by the reactor.

Two preliminary experiments have been performed to avoid the influence of the background radiation. Firstly, the distance between a sample holder and a scintillation detector was reduced to improve the effective ratio of positron annihilation gamma-rays to background gamma-rays. Secondly, an additional circuit to improve an energy resolution of the scintillation detector was installed to cut unwanted gamma-ray signals. A lifetime value of 387 ± 12 ps was obtained for a Kapton film with the second method. This lifetime value was in agreement with the previous studies. Further improvements as well as age-momentum correlation (AMOC) measurements are in progress.

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Positron annihilation in bulk materials by using 17 MeV gamma beam induced positron beam

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We have developed a simple fast positron beam apparatus on the specialized high energy gamma beamline at synchrotron radiation facility "NewSUBARU" in Hyogo prefecture, Japan. This fast positron beam is created from quasi-monochromatic 17 MeV gamma beam directly via pair-creation in a Pb target and energy selection by applying of a magnetic field. By using this apparatus, we have successfully measured the defects and open volume in some bulk materials [1,2]. However, the depth profile of this fast positron annihilation is not well studied. In this study, fast positron annihilation Doppler broadening profiles for stacked iron and silicon plates with various stacking order each other were measured by using this positron beam. From these data, fast positron penetration and annihilation depth profile were estimated. The results of the Doppler profile of fast positron implanted into bulk iron have a good correlation with those of Monte Carlo simulation by PENELOPE code [3].

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Binary-encounter-dipole model for positron impact direct ionization

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Kim and Rudd [1] developed a parameter-free binary-encounter-dipole (BED) model for electron impact ionization of atoms and molecules. They combined the modified Vriens's symmetric binary encounter theory [2] including interference between the direct and the exchange terms and the Bethe theory [3] for fast incident electrons. This model has been shown to be remarkably accurate for ionization of atoms, ions, and molecules [4]. Different modified versions of BED have been proposed in order to expand the applicability of this theoretical approach, see e.g. [5]. However this model has not been tested accurately for positron impact direct ionization so far. BED can be used to calculate positron impact cross sections with simple exclusion of the exchange and the interference terms. The recent progress in the development of positron beam techniques, see e.g. [6] allowed for accurate measurements of positron direct ionization cross-sections. The current database of experimental cross-sections is rich enough in order to carry out comparative studies for semi-empirical models such as BED. In this work the applicability of BED model is tested for positron direct ionization of several targets (H, He, H₂, Ne).

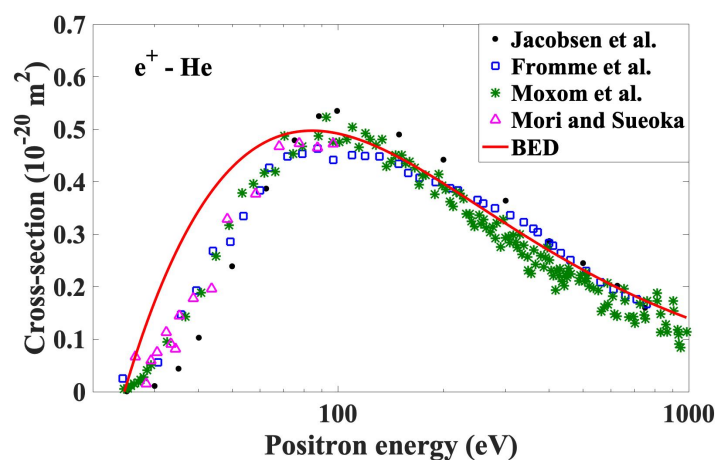


Figure 1 Positron impact direct ionization cross-sections for helium. BED compared with experimental data by Jacobsen et al. [*J. Phys. B: At. Mol. Opt. Phys.* 28, 4691 (1995)], Fromme et al. [*Phys. Rev. Lett.* 57, 3031 (1986)], Moxom et al. [*Can. J. Phys.* 74,367 (1996)], and Mori and Sueoka [*J. Phys. B: At. Mol. Opt. Phys.* 27, 4349 (1994)].

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Oxidation of ScN films and effect on these properties.

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Scandium nitride (ScN) is a rocksalt-structure semiconductor that has attracted attention for its potential applications in thermoelectric energy conversion devices, as a semiconducting component in epitaxial metal/semiconductor superlattices. This material presents a strong sensitivity to the air and can quickly oxidize. ScN layers were deposited onto the surface of MgO (001) substrate at different temperatures. A strong correlation was observed between the oxidation level of layers and the crystallization of films. The shift of the first direct band gap was measured from 2.1 eV and 2.6 eV and can be correlated with the observed change of the carrier concentration. In the best condition of deposition, several thicknesses of ScN varying from 60 nm to 1 μm were deposited. A change in the crystalline orientation of the ScN films was observed as a function of the thickness. Positron measurements were performed to measure the defects concentration in the films induced by this changing. Pulsed positron beam measurements were employed in order to determine the type and the concentration of defects in the films induced by this changing.

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Remarks on R-parameter extracted from DB spectrum related to three-photon annihilation

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Three-photon annihilation process results from the self decay of o-Ps but also from annihilation of a free positron and electron with spins parallel. Usually the observation of three photons was a way to detect such processes, but it is not an effective way, because it requires the convergence of the three, and therefore strong sources. Using HPGe and analyzing the energy spectrum of emitted photons is much simpler. In this case, the three-photon annihilation results in a continuous energy spectrum of emitted photons, which is the opposite of the annihilation of two photons. The so called R-parameter, or peak to valley ratio is the commonly use for characterization of this process. There will be presented some critical comments regarding this parameter, which is sensitive not only to the three-photon annihilation but also to the geometry of measurements. Each factor which affects the photon absorption in the sample or in the environments influence the R-parameter value. Then the interpretation of the data makes a risk even in the slow positron beam experiment. Some examples of typical measurements will be given too.

There will be presented the newest version of the SP code developed for extraction of the S-parameter from the annihilation line, in this version the option for determination also R-parameter from the energetic spectrum was added.

Para-positronium in polymers and silica glass

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It is possible to deduce the S parameter associated with the pick-off annihilation of ortho-positronium (o-Ps) in polymers and SiO₂, providing unique information on the electrons participating in the pick-off annihilation process, by positron-age momentum correlation (AMOC) spectroscopy [1]. In the present study, we attempted to estimate the S parameter relevant to para-positronium (p-Ps) and discuss its implication to the self-annihilation of p-Ps.

From the time dependence of the overall S parameter, $S(t)$, obtained from the AMOC spectra of polymers and SiO₂ reported in [1], the S parameter associated with p-Ps, S_{p-Ps} , was evaluated. In doing so, the lifetime and yield of o-Ps were fixed respectively to the lifetime and relative intensity of the longest-lived component observed for the same materials by positron lifetime spectroscopy. The p-Ps yield was fixed to one third of the relative intensity of the longest-lived component.

Prior to the annihilation, positronium (Ps) in polymers and SiO₂ is thought to localize in a sub-nanometer space. The pick-off annihilation lifetime of o-Ps is determined by the size of this sub-nanometer space. According to the study of silica glasses with different compositions by Angular Correlation of Annihilation Radiations (ACAR) [2], the momentum distribution of p-Ps also depends on the size of the sub-nanometer hole. We compared S_{p-Ps} obtained by AMOC spectroscopy with the S parameter expected for p-Ps localized in a hole and found that they agree with each other for polymers such as polyethylene, polystyrene etc. However, for some polymers and SiO₂ S_{p-Ps} is far less what is expected for p-Ps localized in a hole, suggesting p-Ps annihilating prior to thermalization.

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Controlled drug release monitored by PALS

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Development of new controlled drug release systems for oral application is constantly a topic of interest. The solubility of active pharmaceutical ingredients (APIs) in an aqueous environment is one of the most important factors determining the selection of a strategy to control their release. In the case of water-soluble medicines, the most effective approach is to control the infiltration of the dissolution medium. This can be done by dispersing API in a porous matrix, which results in the formation of a solid dispersion of the drug within the carrier. *In vitro* examination of the API release rate from the solid dispersion to the dissolution medium allows to assess usefulness of the system as the controlled release one [1].

To better understand the course of the drug release positron annihilation lifetime spectroscopy (PALS) was used for the study of the solid dispersion at various stages of the release (Fig.1). On the basis of obtained results, it can be assessed how the microstructure of the carrier-drug system influences properties of the controlled drug release system. Structure examination using PALS was supported with N₂ adsorption and SEM/EDS studies. They allow to determine the parameters characterizing the porous structure as well as the morphology and the spatial distribution of the elements in an examined sample cross-section. A perspective study using positron microbeam seems to allow complementing the SEM/EDS results by position-sensitive PALS and extend information obtained with this technique.

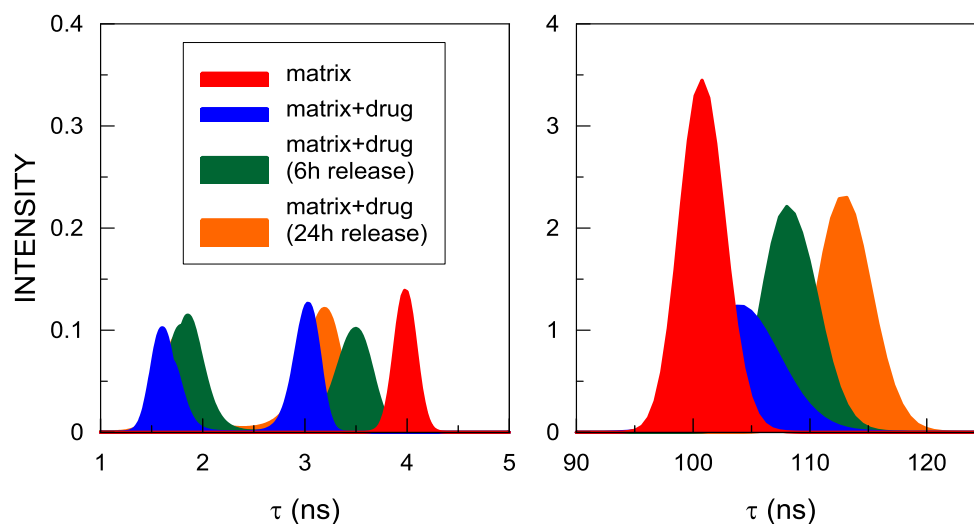


Figure 1 *Ortho-positronium components related to the drug (short-lived) and mesopores (long-lived) in the porous matrix and the matrix-drug composite at various stages of drug release.*

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Estimation of the effect of positron production amount by installing Cd-cap in the KUR slow positron beamline

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As well as other reactor-based positron beam facilities [1–3], a Cd-cap is used in the slow positron beamline at Kyoto University research Reactor (KUR) in order to enhance the gamma-ray intensity irradiated to a tungsten positron converter [4]. During KUR maximum power operation (5 MW), the temperature around the Cd-cap reaches up to several tens of degrees below the melting point of Cd (321°C) due to nuclear heating. The Cd-cap-installed beamline requires extra attention and/or effort due to the low melting point material. Thus, to estimate how much the Cd-cap contributes to positron production is important for reactor-based positron beam facilities. In this study, the change of positron production amount with and without the Cd-cap at the KUR beamline was estimated by Monte Carlo simulation.

Figure 1 shows the change in the amount of positron emission from the tungsten positron converter with and without the Cd-cap, assuming that only neutrons are emitted from the reactor core. In the calculation, the structure of the positron production unit of the KUR beamline shown in Fig. 2 was modeled as truly as possible including reactor coolant water. Since gamma-rays derived from neutrons are also emitted from materials around the converter, positrons are produced to some extent even without the Cd-cap as shown in Fig. 1. However, the amount of positron emission was found to increase 6.0 ± 0.2 times by installing the Cd-cap. Although the above calculation considers only neutrons, in fact, gamma-rays emitted from the reactor core also contribute to positron production. In the presentation, the change in the total amount of positron production with and without the Cd-cap will be discussed.

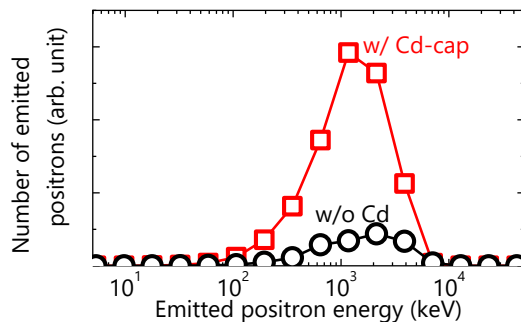


Figure 1 The number of emitted positrons from a tungsten positron converter as a function of emitted positron energy. Note that only neutrons are considered in this calculation.

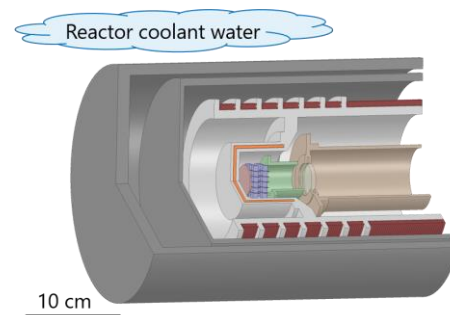


Figure 2 Schematic diagram of positron production unit of the KUR beamline. Note that this is not the model used in the calculation.

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Development of the J-PEM for breast cancer detection and diagnosis using positronium imaging

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A detection system of the conventional PET tomograph is set-up to record data from e^+e^- annihilation into two photons with energy of 511 keV, and it gives information on the spatial density distribution of a radiopharmaceutical in the body of the object [1].

Our goal is to design, construct and to establish the characteristic performance of the J-PEM (Jagiellonian Positron Emission Mammography), which is imaging modality for the detection and diagnosis of breast cancer, based on a novel idea with plastic scintillator [2,3] and wavelength shifter (WLS) [4]. Out of all imaging modalities, J-PEM is a type of Positron Emission Mammography (PEM) which is a dedicated and well-recognized technique to diagnosis the breast cancer which is based on the same principle as that of PET.

J-PEM can be an effective system for the detection and diagnosis of breast cancer in its early stage by improving sensitivity and specificity and it can be achieved by the combined use of plastic scintillators, which have superior timing properties, with the WLS. In addition this device will be developed in view of classification of malignancy based on the possibility of positronium mean lifetime imaging [1].

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Progress towards a magnetically confined electron-positron pair plasma

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The APEX collaboration is aiming to magnetically confine a low-temperature electron-positron pair plasma [1] in a levitated superconducting coil. Such pair plasma represents a unique state of matter whose experimental realization is still pending.

In a prototype magnetic dipole trap the basis for the realization of a laboratory pair plasma is provided. Positrons from the NEPOMUC facility at FRM II near Munich are guided towards this confining device. It consists of a supported, cylindrical permanent magnet, surrounded by a cylindrical set of ten electrodes. These electrodes are segmented and can be biased individually either by applying static or time varying potentials. To inject positrons into the confining magnetic field, a drift across magnetic field lines is required. We induce this process by a pair of ExB plates, placed at the injection port. Extensive investigations of the large parameter space spanned by the conceivable electrostatic and magnetic field configurations deepened the understanding of the injection process and resulted in injection efficiencies of 100% [2] and positron confinement times exceeding one second [3].

As a next step towards a mixed state of positrons and electrons, a compact electron gun placed upstream the beam line creates an electron beam propagating parallel to the positron beam. It was demonstrated that both electrons and positrons can be injected into the confinement volume simultaneously by using the parameters originally optimized for efficient positron injection. For diagnostics, both the annihilation counts of positrons as well as the electron current are measured. Eventually we aim to magnetically confine an electron-positron pair plasma using a levitated superconducting coil. Injecting this two-species mixture simultaneously into the confinement volume is an important step towards this goal. In this contribution the aforementioned milestones as well as future prospects of the APEX project will be discussed.

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Measuring long lifetimes with DRS4 and QtPALS

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Digital PALS setup with switched capacitors array, based on affordable DRS4 evaluation board and QtPALS[1] software has been used on a daily basis since 2014 in our laboratory. Setup is used mostly for the measurement of metallic samples. In such case, positron annihilation bulk lifetimes are in the area around 100 ps with defect lifetimes around 200 - 400ps. For this measurement time axis within 10 – 20ns is adequate. In other applications, for instance, chemistry [2], longer lifetimes are measured, and the used time axis needs to be longer. For this purpose, DRS4 possibilities with using maximum allowed time window and lower sampling rates were tested and evaluated. In the process of the long times measurement tests, spectra distortion was observed. Source of this distortion and solution on how to eliminate it will be explained.

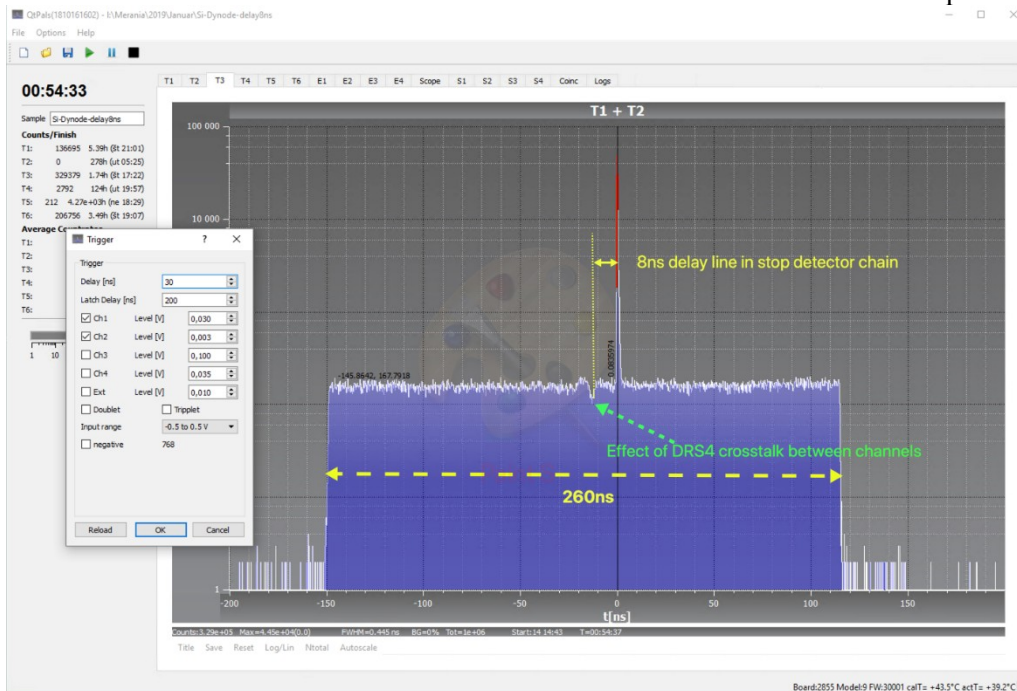


Figure 1 Maximising of the time axis by latch delay settings in QtPALS and spectra distortion caused by signal crosstalk.

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Investigation of Optical Properties and Defects Structure of Rare Earth (Sm, Gd, Ho) Doped Zinc Oxide Thin Films Prepared by Pulsed Laser Deposition

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In past decades a lot of efforts have been put in fabrication of high quality ZnO thin films. Such films of low defects concentrations can serve as a part of several optoelectronics devices (waveguides, LEDs, solar cells and sensors). The optical properties can be tuned and enhanced by doping ZnO with rare earth (RE⁺) elements up to 3 at. %. Strong emission lines in ZnO:RE structures can be obtained in visible and infrared spectral region.

Pulsed Laser Deposition (PLD) has been shown as promising technique for fabrication of thin films of complex structure. ZnO films prepared by PLD exhibit typically oxygen deficiency leading to enhanced concentration of oxygen vacancies. Deposition in oxygen enriched atmosphere can eliminate this problem and eventually create Zn vacancies.

ZnO:RE thin films were grown by PLD (Nd:YAG, $\lambda = 266$ nm, $\tau = 6$ ns) from ZnO:Sm₂O₃, ZnO:Gd₂O₃ and ZnO:Ho₂O₃ targets (RE content was 1 at. %) in oxygen ambient at pressure of 5, 10 and 20 Pa on fused silica and Si (100) substrates at room temperature. Defects structure was examined by variable energy positron annihilation spectroscopy (VEPAS). Doppler broadening of annihilation radiation was evaluated using S and W line-shape parameters as a function of energy of implanted positrons. Morphology of the films was characterized by atomic force microscopy. The optical properties were analysed by spectrophotometry, spectral ellipsometry and photoluminescence.

Electrotransport properties were characterized by resistivity measurements.

All ZnO:RE films exhibited significantly higher values of the S parameter as well as shorter positron diffusion lengths compared to ZnO monocrystal reference due to nanocrystalline structure of the films as was observed by AFM. We assume positrons were predominantly trapped at grain boundaries.

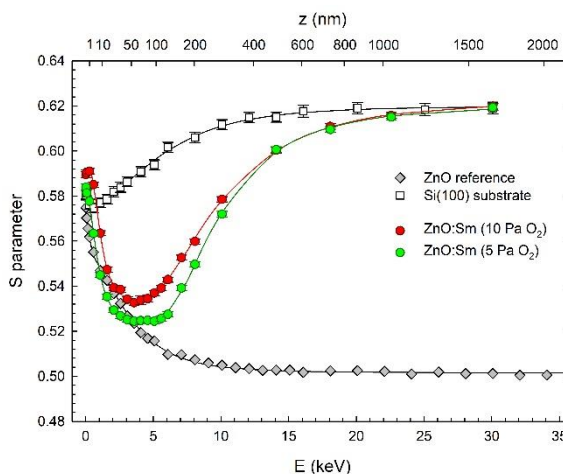


Figure 1 S(E) curves for ZnO:Sm films prepared under 10 Pa and 5 Pa O₂ atmosphere, reference curves of the Si substrate and ZnO reference are included.

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A supervised Machine Learning Approach for Shape sensitive Detector Pulse Discrimination in Positron Spectroscopy Applications

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The acquisition of high-quality positron spectra is crucial for a profound analysis, i.e. the correct decomposition to obtain the *true* parameters. Since the introduction of digital spectrometers for the techniques of PALS and CDBS, this is generally achieved by applying various (software-based) filters/corrections on the digitized output-pulses from photomultipliers/HPGe-detectors prior to spectra generation. For instance, pile-up events can be easily detected and subsequently rejected by applying pulse-area/shape sensitive filters, which significantly increases the peak-to-background ratio.

Here, we present a novel approach for shape-sensitive discrimination of detector output-pulses using supervised machine learning (ML) based on a simple probabilistic classification model: the *naive Gaussian Bayes classifier*. In general, *naive Bayes* methods find wide application for many real-world problems such as famously applied for email spam filtering, text categorization or document classification. Their algorithms are relatively simple to implement and, moreover, perform extremely fast compared to more sophisticated methods in *training* and *predicting* on high-dimensional datasets, e.g. detector-output pulses.

We compared the quality and decomposability of lifetime spectra acquired on pure metals from a single measurement (pulse stream): (1) generated by applying the ML approach (software: `pyDMLDetectorPulseDiscriminator` [1]) to lifetime spectra generated using `DDRS4PALS` software (2) with and (3) without filters applied [2].

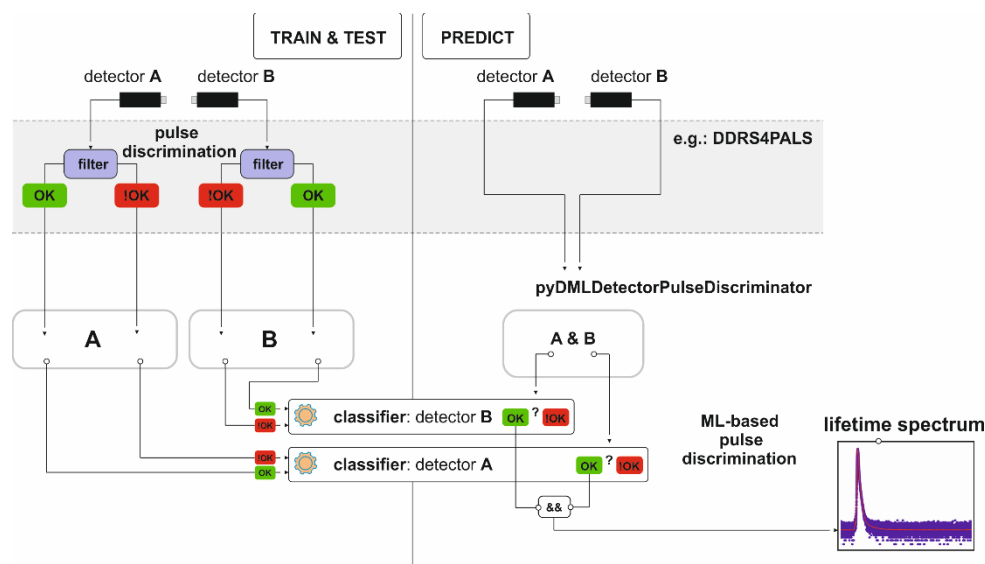


Figure 1 Basic principle of the here presented supervised machine learning (ML) approach for shape-sensitive discrimination of detector output-pulses for the technique of PALS.

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Data-scientific software for the surface structure analysis by total-reflection high-energy positron diffraction (TRHEPD)

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The data scientific software was developed for the surface structure analysis by the total-reflection high-energy positron diffraction (TRHEPD). The experiment has been intensively conducted at the Slow Positron Facility (SPF), Institute of Materials Structure Science (IMSS), High Energy Accelerator Research Organization (KEK) and revealed the structure of the surfaces of interest [1].

The present paper reports the recent activity of the software development for the data analysis of TRHEPD. It is based on the inverse problem in which the atomic positions $X = (X_1, X_2, \dots, X_N)$ of a surface structure are determined from the experimental diffraction data (rocking curve) D_{exp} ($D_{\text{exp}} \Rightarrow X$). The forward problem ($X \Rightarrow D_{\text{cal}}(X)$) is solved, for many trial atomic positions X , by the numerical solution of the partial differential equation in quantum scattering problem [2]. The R-factor $R(X) = |D_{\text{cal}}(X) - D_{\text{exp}}|$, the residual error between the experimental and calculated diffraction data, is minimized as a function of the atomic position. Two possible methods are considered; one is the local search procedure by the gradient-free optimization (Nelder–Mead) method and the other is the global search procedure by the grid or stochastic sampling (Monte Carlo) method. The global search procedure requires a large computational cost and is realized on supercomputers with parallel computation.

This presentation demonstrates the application of the method to several known surface structures, as preliminary attempts. Our data-scientific approach is general and applicable to other experiments also, like Low Energy Electron Diffraction (LEED), when one replaces the forward problem solver. The program code is written mainly in the Python language and will be available online in near future.

Acknowledgement: The present research is supported by Japanese government in the post-K project and KAKENHI funds (19H04125, 17H02828). Several numerical computations were carried out by the supercomputer Oakforest-PACS for Initiative on Promotion of Supercomputing for Young or Women Researchers, Information Technology Center, The University of Tokyo, the HPCI project (hp190066) and Interdisciplinary Computational Science Program in Center for Computational Sciences, University of Tsukuba. Several computations were carried out also on the facilities of the Supercomputer Center, the Institute for Solid State Physics, the University of Tokyo and the Academic Center for Computing and Media Studies, Kyoto University.

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Limitations on the Lifetime Spectra Decomposability applying the Iterative Least-Square Reconvolution Method with the Instrument Response Functions (in)directly obtained from 207-Bi and 60-Co

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The knowledge of the lifetime spectrometer's *instrument response function* (IRF), also known as the *resolution function*, is crucial for a profound analysis, i.e. the correct decomposition to obtain the *true* information: the characteristic lifetimes and its corresponding contributions. The IRF is commonly modelled by a superposition of Gaussian distribution functions since an analytical solution for the convolution with an exponential distribution function exists. Therefore, the acquired lifetime spectra can be described in total as an analytic function and, hence, the least-square fitting can be easily applied, as it was first shown by Kirkegaard and Eldrup in 1972 [1].

However, the *iterative least-square reconvolution approach* [2] determines the best fit of the recorded lifetime spectrum by *re-convoluting* a sum of N expected exponential distribution functions with an experimentally obtained IRF. For a laboratory setup, two variants are well-known to determine the IRF from experiment: the direct method using 60-Co and the indirect method applying 207-Bi. For both methods, the energies of the gamma-rays are considerably shifted from the energies accompanying the creation (1274keV) and annihilation (511keV) of a positron using 22-Na: 60-Co (1170keV, 1330keV), 207-Bi (570keV, 1064keV). Therefore, significant deviations in the retrieved information can be observed, since the IRF strongly depends on the energy deposited in the scintillation material. Even an additional (de)convolution with an empirically chosen Gaussian function (FWHM) mapping/adjusting the energies of the used isotopes, indicates no farther improvements in terms of spectra decomposability.

Here we present a detailed study regarding the spectra decomposability by using the reconvolution approach with the IRFs (in)directly determined from two isotopes: 60-Co and 207-Bi. We can show that not only the width (~FWHM) of the IRF but also the shape of the IRF indicate differences from the true underlying IRF and, thus, an analysis using the reconvolution method is almost impossible to apply.

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Experimental study of light emission during positronium formation in matter exposed to slow positron beam

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Positronium atom (Ps) is formed in matter when a quasi-free electron and a positron diffuse into a free volume nearby. During the Ps formation, an excess of energy can be released and one of the ways of it is photon emission. Here, we present the result of experimental measurements of light emission in coincidence with positronium formation in the case of the samples of octacosane (n-alkane) and a porous silica exposed to a slow positron beam. Both the number of photons and their time of appearance were analysed.

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Frequency stabilisation of high power RF resonators for pulsed positron beams

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To investigate inhomogeneous defect distribution by positron annihilation lifetime spectroscopy a pulsed and focused positron beam is needed. For this purpose the Scanning Positron Microscope (SPM) was built and operated by the Universität der Bundeswehr München [1]. To overcome the limitation of low count-rates obtainable with a laboratory source the SPM is currently transferred to the intense positron source NEPOMUC at the MLZ in Garching [2].

To convert the continuous NEPOMUC beam into a pulsed beam of high brightness a special interface was built [3]. A sophisticated beam preparation is needed to reach a lateral resolution in the micro-meter range. An essential component of the interface is the positron elevator which compensates for the energy loss caused by the remoderation process without altering other important beam properties [4, 5].

The bunching system of the interface works at 50 MHz. This is also the resonance frequency of the resonator. The resonator provides a 10 kV sine-wave at an electrical power of 80 W for the positron elevator. To ensure proper operation of the whole system, stable amplitude, stable frequency and stable phase of the RF-signal are crucial. This is achieved by a newly developed feedback controller.

In this contribution we will give an overview of the complete device with a focus on the frequency stabilization system of the positron elevator, shown in Fig. 1.

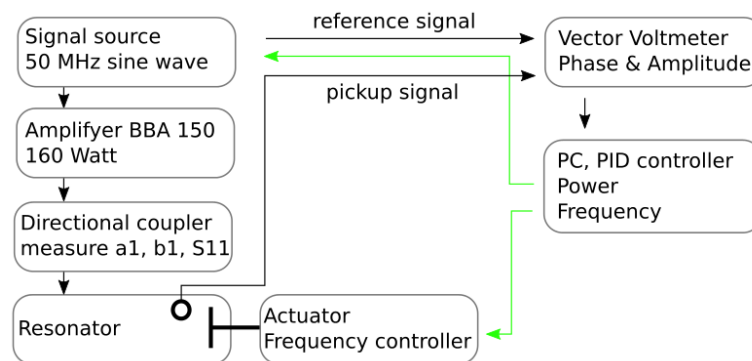


Figure 1 Circuit diagram of the electrical components of the positron elevator.

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Present Status of the Slow Positron Facility of Institute of Materials Structure Science, KEK

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Recent results of the experiments at SPF at IMSS, KEK are reported.

At the total-reflection high-energy positron diffraction (TRHEPD[1.2]) station on the branch SPF-A3, the structure of germanene on Al(111) surface was determined to be different from that previously reported [3]. The structure of Ca-intercalated bilayer graphene is also determined to be different from that previously proposed [4]. Azimuthal analysis, proposed for RHEED [5] before, is being developed, where the azimuthal angle dependence of the spot intensity is analyzed with the glancing angle fixed.

On the branch SPF-A4, The first version of the LEPD (low energy positron diffraction) station was completed, and the incident energy dependence of the LEPD pattern on the Ge (001)-c (4×2) surface was measured [6]. The station is being further improved to make an electrostatic lens 2.5 times longer in order to reduce the background due to the annihilation γ rays from the remoderator, and to implement a hexanode DLD detector.

At the general-purpose station on the branch SPF-B1, experiments of laser cooling of positronium (Ps) as a first step of the realization of Ps Bose-Einstein condensate started. The beam line was modified and the chamber for the positronium negative ion (Ps^-) was replaced with one for the new experiments.

At the positronium time-of-flight (Ps-TOF) station on the branch SPF-B2, temperature dependence of positronium formation at Si(111) and Si(001) surfaces has been investigated by changing the doping levels systematically over the temperature range of 300–1000 K[7]. The Ps-TOF spectra show a component of Ps formed through the work-function mechanism and one through the surface-positron-mediated process.

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Improved defect spectroscopy by in situ light illumination and electric field variation at PLEPS

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The **Pulsed Low Energy Positron System PLEPS** at the intense positron source NEPOMUC at the FRM II in Munich allows to measure positron lifetime spectra using a monoenergetic positron beam of variable energy between 0.5-20 keV [1]. PLEPS is a unique tool to investigate open volume defects in a large variety of material systems, e.g. in wide band-gap semiconductors or in thin-layer structured semiconductors and insulators [2-4].

Defect identification in semiconductors and insulating materials is a challenging task: One encounters a wide variety of different defect types, often with very similar positron lifetimes. The defects may have different charge states, negative, neutral or positive. In addition, samples may contain (multiple) thin layers, interfaces or internal surfaces, which can be narrower than the positron implantation profile.

To meet the challenges for defect identification in those ever more complex materials several modifications of PLEPS are necessary: To change the charge state of defects by illumination a broad bandwidth arc-lamp in combination with a filter system which covers a spectral range from 0.2-2.5 μm will be installed at PLEPS. Electrical fields affect the positron motion in materials and can be used, e.g. to drive positrons towards or away from interfaces [5]. To apply electrical fields to the sample and to measure and manipulate currents and voltages during positron lifetime measurements, a new type of sample holder is currently developed, the sample target station has to be mechanically modified and electrically adapted.

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Positron Annihilation With Quantum Monte Carlo

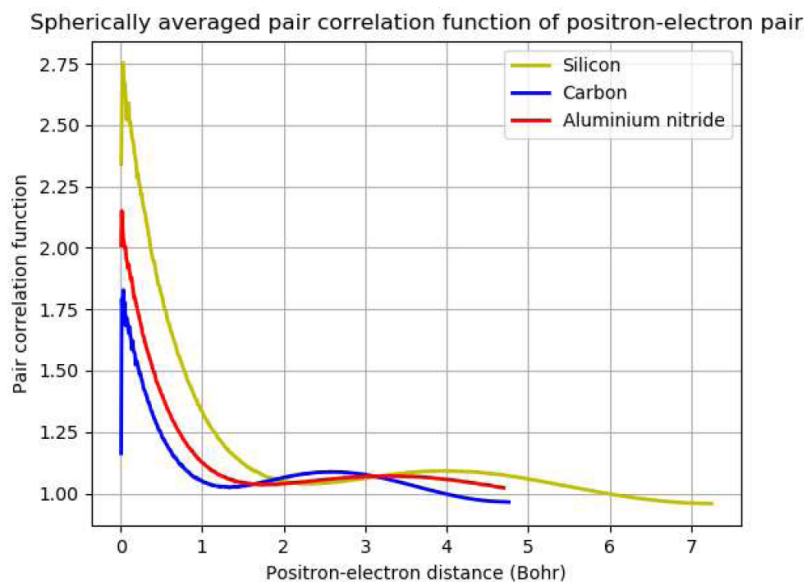
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Experimental use of positron annihilation spectroscopy requires a strong theoretical background for drawing conclusions from the measurements and making a link between the atomic structures of the defects detected and the indirect information in the measured spectra. The most widely used method for making theoretical simulations of positron annihilation is density functional theory (DFT) [1]. While it is proven to be highly practical, there is demand for more accurate methods. This is why we have developed a Quantum Monte Carlo (QMC) [2] method for simulating positrons in solids. QMC does not require the approximation of multiple functionals, and it is able to sample directly two-body quantities, as well as expectation values in the momentum space. The trial wave functions are in a localized blip basis. With QMC, the electron-positron wavefunction is first optimized with variational Monte Carlo method (VMC), after which it is passed forward for the extremely accurate diffusion Monte Carlo simulation (DMC).

At the moment, we have obtained accurate predictions of the lifetimes of positrons in diamond phase-carbon and -silicon and wurtzite aluminium nitride. We are also studying correlation between electrons and a positron in the crystals as a function of location in real space by sampling enhancement factors, and examining how correlations play a role in annihilation events. In the future we may also simulate the Doppler broadening spectrum of annihilating electron-positron pair.



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Multi-Functional Positron Beam for the Coincident Measurement of the Energy Spectra of Doppler-Shifted Annihilation Gamma Quanta and Positron Annihilation-Induced Electrons

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Preliminary results are presented which were collected using a new positron beam system at the University of Texas at Arlington (Figure 1). The beam allows for the coincident measurement of the energy of Doppler-shifted annihilation quanta and time-coincident positron-induced electrons. Previous apparatus have allowed for the coincident measurement of the energies of annihilation gamma rays and annihilation-induced Auger electrons, but only for electrons emitted into a narrow range of energies [1]. The system reported here allows for the parallel collection of a 2-dimensional array of coincident pairs of gamma and electron energies over the full energy range of relevance. The array is constructed from a digital analysis of the pulses resulting from the detection of electrons by a micro-channel plate in coincidence with the pulses resulting from the detection of associated annihilation gamma rays. The system can be used with a NaI (Tl), BaF₂, or HPGc gamma detectors depending on the experiment. Additionally, in-house developed software permits the system to acquire multi-electron spectra, allowing for the observance of multi-electron processes.

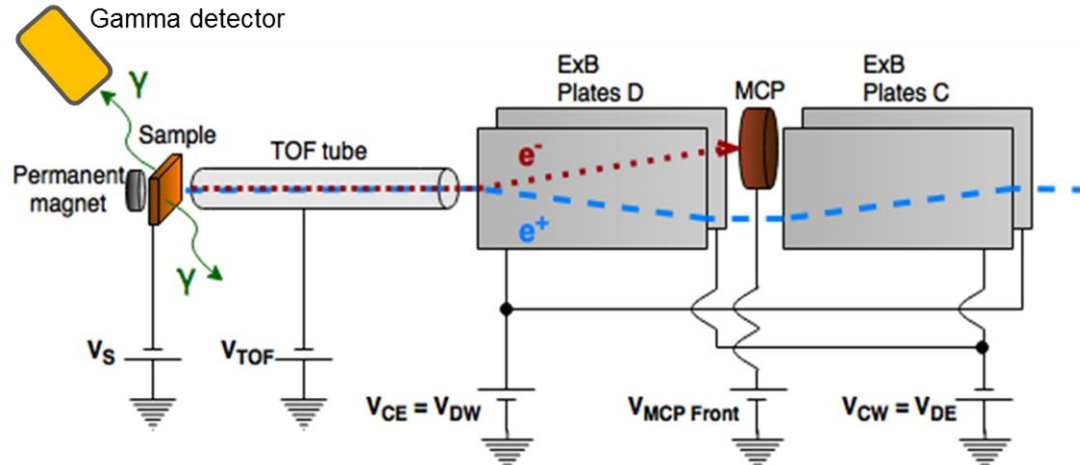


Figure 1 Schematic of the inner ion optics of the positron beam apparatus displaying the paths of the positron beam and resulting positron-induced electrons from the sample surface. The type of gamma detector can be interchanged depending on the type of experiment.

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Positron annihilation induced Auger electron spectroscopy (PAES) measurements of a TiO₂(110) surface

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Recently Tachibana et al. [1] found that positron induced O⁺ desorption (e⁺SD) from TiO₂ was enhanced in comparison to electron induced O⁺ desorption for incident particles in the energy range from 10 eV to 600 eV. They proposed that this enhancement was due to the annihilation of surface trapped positrons with inner shell electrons [1]. Here we report measurements of positron induced electron emission from a TiO₂(110) surface which may provide insights into the desorption process. The energy of the positron induced electrons were measured using its time of flight, which is taken as the time difference between the detection of the annihilation gamma and the positron induced electron. The positron induced electron spectrum [Fig.1] exhibit relatively narrow peaks at ~ 260 eV and ~ 500 eV corresponding to Auger transitions initiated by the annihilation of 1s electrons in carbon and oxygen respectively. The most significant feature of the spectrum is a broad low energy peak extending from ~ 2 eV to ~ 15 eV. Since the incident positron beam energy (3 eV) was well below the energy necessary to directly knock out electrons of these energies, the peak must be due to an annihilation induced process. The origin of this low energy peak in terms of Auger processes resulting from the annihilation of positrons with deep valence and shallow core levels in TiO₂, and the possible importance of such processes to e⁺SD will be discussed.

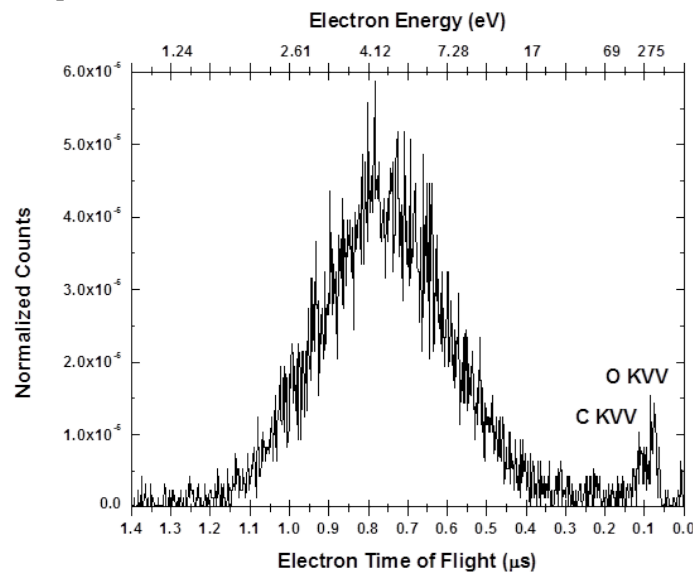


Figure 1 Positron annihilation induced Auger electron spectrum (PAES) from a TiO₂(110) surface. Core KVV Auger peaks corresponding to 1s Auger transitions in carbon and oxygen are present alongside a broad low energy peak. This spectrum was measured using a positron beam energy of 1 eV and a sample bias of -2 V.

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Doppler broadening spectra from multilayer graphene on copper

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We present the Doppler broadening spectra measured from six to eight layers of graphene on Cu using an advanced positron beam system developed at the University of Texas at Arlington. Sample surface may be considered as a large defect and hence the gamma spectrum originating from the annihilation of surface trapped positrons may be different from the gamma spectrum originating from the annihilation of positrons from a defect-free bulk of the same sample. This may make it difficult to analyze and deduce the chemical architecture of the sample surface from the surface annihilation line shape as most of the calculated and experimental spectra in literature [1] are from bulk samples. Therefore, a systematic investigation of the Doppler spectrum from surface state annihilations is warranted. In order to obtain positron annihilation almost exclusively from the surface, experiments were performed using low energy positrons (~ 2.0 eV). It has been shown previously [2] that, at these low energies, positrons trap and annihilate in the surface state of the sample which in this case is graphene. The ratio of the Doppler broadened gamma spectrum collected at a positron beam energy of 2 eV (surface) to that collected at 20 keV (mainly bulk Cu) (Fig.1 (a)) was compared to a theoretically calculated ratio curve obtained by taking a ratio of the calculated Doppler spectrum for the bulk graphitic Carbon to the calculated Doppler spectrum for bulk Cu (Fig. 1(b)). The experimental ratio curve is different from the theoretical ratio especially at low momentums. However, there is an agreement in the high momentum region ($> 0.015 m_0c$), which shows that surface annihilations can be used to deduce chemical information from the top most atomic layer. We will discuss the above results by comparing the shape of the experimental ratio curve to the theoretical ratio curve obtained for individual electron orbitals of bulk graphitic carbon.

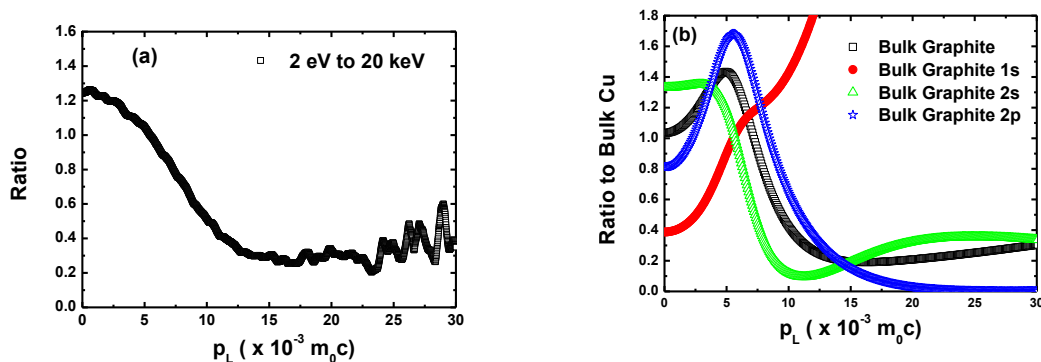


Figure 1 (a) Doppler broadened gamma spectra from the surface of 6-8 layers of Graphene (2 eV) divided by the Doppler broadened spectrum from bulk Cu (20 keV) (black squares). (b) Ratio curve obtained by dividing the theoretically generated Doppler broadened spectrum from bulk graphitic carbon and various electron orbitals in carbon to that obtained from bulk Cu.

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Effect of oxygen pressure on optical and electrical properties of single-crystalline Cu₂O fabricated by pulsed laser deposition

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Copper oxide Cu₂O is an important and well known p-type transition metal oxide semiconductor material which has the advantages of direct band gap 2.1 eV and high absorption coefficient in the visible spectral range. This material has already been employed in the fabrication of electronic devices, thanks to its low cost, non-toxicity and fairly good carrier mobility. For example Cu₂O has been used in thin photovoltaic devices, resistive switching, transistors, gas sensors or catalysts.

In our work the epitaxial films Cu₂O (110) have been fabricated by Pulsed Laser Deposition on MgO(100) substrates maintained at temperature 700°C. Our attention was focused on the influence of the oxygen pressure, which was varied between 10⁻⁵ Pa and 10⁻¹ Pa, on the structural and following on optical and electrical properties. The crystalline quality and out-of-plane orientation of the films were characterized by means of X-ray diffracton. The surface morphology and composition were characterized by Atomic Force Microscopy and XPS, respectively. The optical properties, complex dielectric constants, and optical gap, of the films were determined by spectral ellipsometry in the range of 250 - 1700 nm. Resistivity and Hall voltage measurements were carried out using the differential van der Pauw (vdP) method in a quasi-square arrangement at room temperature.

Because of Cu₂O is a natural p-type semiconductor, whose carrier concentration depends on copper and vacancies, our attention was focused on the examination of defects by means of Electron paramagnetic resonance (EPR) and Positron annihilation spectroscopy (PAS). EPR carried out in the temperature range from 5K to 700 K on Bruker ELEXSYS E580 at X-band. PAS measurement of Cu₂O films was carried out on a pulsed slow positron beam MePs at the Electron LINAC with high Brilliance and low Emittance (ELBE) facility at Helmholtz Zentrum Dresden-Rossendorf. The energy of incident positrons was varied in the range from 1 to 16 keV.

Two exponential components corresponding to positron annihilation in Cu₂O layer were resolved in lifetime spectra: (i) positrons trapped at vacancies and (ii) large vacancy clusters with lifetime $\tau_2 = 400$ ps to 500 ps. The sample deposited under high oxygen pressure contains predominantly single copper vacancies V_{Cu} ($\tau_1 = 229$ ps) while the sample deposited under low oxygen pressure contains complexes of copper vacancies coupled with oxygen vacancies ($V_{Cu} + V_O$ and $V_{Cu} + 2V_O$, $\tau_1 = 262$ ps and 284 ps) due to the oxygen deficiency during the deposition. Since isolated oxygen vacancy is not able to trap positrons, it cannot be detected by positron annihilation spectroscopy. The sample deposited under low oxygen atmosphere contains bigger vacancy clusters compared to the sample deposited under high oxygen pressure.

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Characterization of small-scale samples using radioisotope positron sources

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Probing of small-scale samples such as thin ion-implanted layers or TEM discs using conventional encapsulated positron sources is usually complicated by positron annihilation outside the inspected volume. Besides, experimental spectra obtained from samples containing internal transmutation-based positron source are naturally disturbed by positron emission outside of the sample. To estimate these contributions to the spectra, Geant4 simulation toolkit was used. In addition to various absorption profiles of positrons from realistic encapsulated sources, the applicability of the use of TEM disc containing $^{44}\text{Ti}/^{44}\text{Sc}$ [1] as external positron source is reviewed.

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Effects of Magnetic Non-adiabaticity and Measurement of the Energy Distribution of a Solid Neon Moderated Positron Beam*

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High quality, trap-based positron beams typically operate in the regime in which particle transport is adiabatic. In this regime, the quantity (E_{\perp}/B) is a so-called adiabatic invariant (AI), where E_{\perp} is the energy in cyclotron motion in the direction perpendicular to magnetic field B . Adiabaticity requires the parameter $\gamma = (2\pi v_{\parallel}/\omega_c) (1/B)(dB/dz) < 1$, where ω_c is the cyclotron frequency and v_{\parallel} is the parallel positron velocity [1].

Discussed here is a positron beam from a ^{22}Na source and a cone-shaped solid neon moderator. For all beam transport energies ≤ 100 eV, invariance holds quite well for the beam from the buffer gas trap (BGT) to the test-gas cell [2]. However, upstream of the BGT, breaking of AI is observed for transport energies ≥ 60 eV. This has been identified to be due to the low magnetic field and strong gradients at front end of the beam tube separating the solid-Ne moderator source stage and the BGT. The principle effect of the breaking is that it scrambles the parallel (E_{\parallel}) and perpendicular energy (E_{\perp}) beam distributions, leading to broadening of both, while the total particle energy is conserved. Experimental results for a fixed source magnetic field show increases in mean perpendicular energy with increased moderator bias in the range 60 – 80 V, in the regime where $\gamma \geq 1$.

The result of these studies is that the mean total energy of the positrons from the solid neon moderator could be measured with the result that, in the adiabatic regime, mean $E_{\perp} \sim 0.8$ eV, mean $E_{\parallel} \sim 1.6$ eV (relative to the moderator bias), and the parallel energy spread is ~ 2 eV FWHM. Measurement of the spatial distribution of positrons from the cone-shaped surface of the neon moderator will also be discussed, as will implications of these observations for BGT-based beam systems.

* Work supported by the U. S. NSF, grant PHY-1702230.

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New Measurements of Positron Annihilation on Molecules*

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Experiments have shown that low-energy (sub-eV) annihilation spectra of positrons on molecules are typically dominated by relatively sharp features that have been identified as vibrational Feshbach resonances (VFR) involving fundamental modes [1]. Further, in most molecules there is a broad spectrum of enhanced annihilation between the fundamentals, in the region of combination and overtone vibrational modes, where the density of modes is typically too high to identify discrete modes [2]. Ultimately, the experimental resolution of the spectrum is dependent on the energy resolution of the positron beam. Over the last several years, we have made a number of advancements in understanding the factors limiting the energy resolution of trapped based positron beams [3].

Several experiments will be described, including new measurements of positron binding energies for several alkane molecules with chlorine or oxygen substitutions. Also, annihilation spectra are compared for rings and chains using a room-temperature buffer-gas trap-based beam with improved energy resolution. It reveals anomalous broadening of the VFR structure for the ring geometry. We will describe the status of our cryogenic buffer-gas trap-based beam, which has the capability to increase the energy resolution by a factor of five [4]. Lastly, we will discuss the possibility of clarifying the role of combination and overtone modes in producing the broad background observed in positron annihilation spectra as a function of incident positron energy [5].

* Work supported by NSF grant PHY-1702230.

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Angle resolved ($e^- + H_2O$) measurements near 0°

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A fully electrostatic beam [1] characterized by a high angular discrimination ($\approx 0.7^\circ$) has been used to measure the total (σ_T) and differential cross section of e^- scattering from water vapor. Measurements for σ_T have previously been carried out on the same equipment for $e^+ + H_2O$ [2].

Although cross sections for electron systems have been investigated since the early 20th century, discrepancies had remained among experimental and theoretical results at low energies until now e.g. [3, 4]. The new results for σ_T [5] are presented in figure 1, together with previous experimental and theoretical determinations. The effect of forward scattering has also been probed in the angular range $0 - 3.5^\circ$ and measures of the average (rotationally and vibrationally summed) differential elastic cross sections for energies ≤ 12 eV have been obtained at a scattering angle $\approx 1^\circ$ [5]. These measurements provide the first test of theoretical predictions in an angular region experimentally unexplored until now.

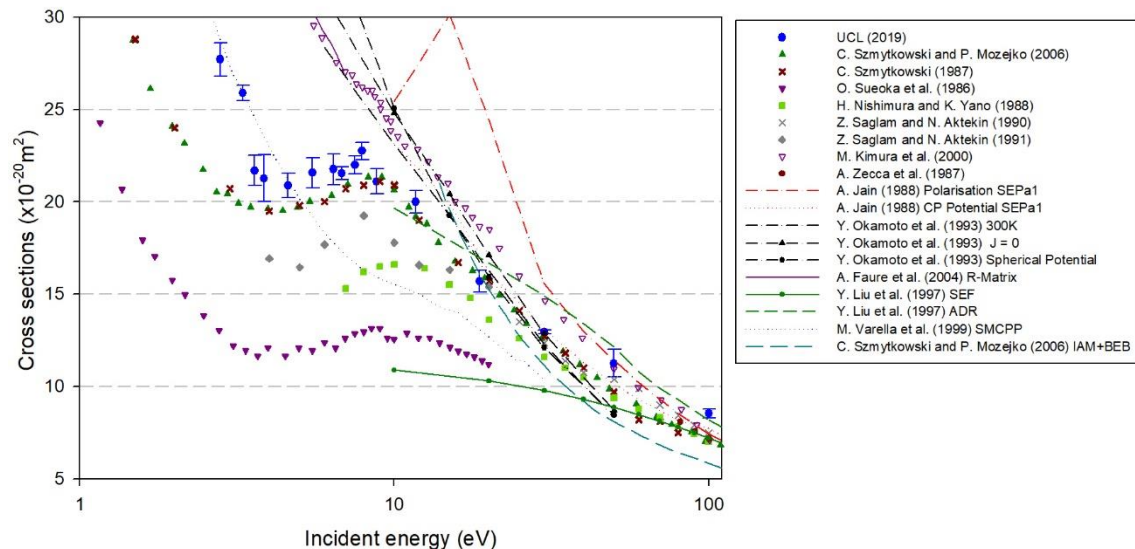


Figure 1 Experimental and theoretical cross sections for electron scattering from H_2O . Solid symbols denote direct measurements, hollow symbols denote measurements corrected for forward angle elastic scattering and lines denote theories [5].

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Defects in thin layers of high entropy alloy HfNbTaTiZr

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High entropy alloys exhibit various combinations of interesting physical properties due to the formation of solid solution stabilized by high configurational entropy. High entropy alloy HfNbTaTiZr exhibit one phase solid solution with BCC symmetry when prepared by arc melting [1]. It was found that this alloy exhibits relatively high absorption capacity of hydrogen and fast kinetics of hydrogen absorption and desorption. Hydrogen diffusion may be enhanced by suitable open volume microstructure. Therefore, pulsed DC magnetron sputtering at room temperature was performed to obtain amorphous layer consisting of homogeneously distributed elements. Very fine microstructure of nanoscale grains was observed by SEM and AFM methods. Therefore, very high concentration of defects is expected to be present in sputtered films of HfNbTaTiZr. Slow positron beam was used to examine the nature of defects associated with layer growth.

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Quenched-in vacancies and hardening of Fe-Al intermetallics

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Physical properties of Fe–Al intermetallics are strongly influenced by the atomic ordering and point defects. During cooling from high temperatures Fe–Al alloys with Al content in the range 30–50 at.% undergo ordering from the disordered A2 phase to the partially ordered B2 structure. Fe–Al alloys with lower Al content 22.7–30 at.% undergo also a phase transition from the disordered A2 phase to the partially ordered B2 phase, but ordering continues with decreasing temperature and the B2 structure is transformed into the ordered D0₃ phase. As shown in Fig. 1b hardness of Fe–Al alloys shows a non-trivial dependence on chemical composition and cannot be fully explained by consideration of intermetallic phases formed. This is due to additional hardening effect by quenched-in vacancies. The concentration of vacancies was estimated from positron back-diffusion measurement on a slow positron beam (see Fig. 1a) and was found to strongly increase with increasing Al content. Comparison of vacancy concentration and hardness revealed that hardening of alloys with low Al content (< 30 at.%) is caused predominately by anti-phase boundaries while vacancy hardening dominates for alloys with higher Al content (above 30 at.%)

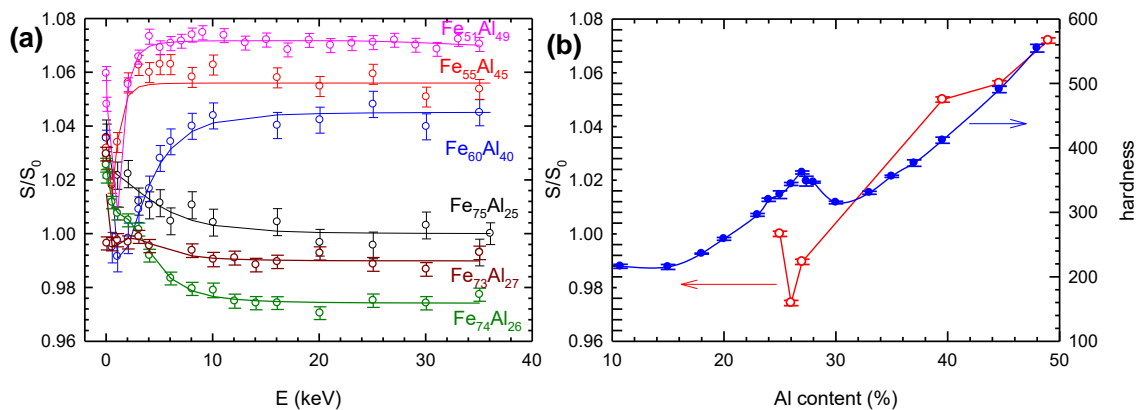


Figure 1 (a) $S(E)$ curves for Fe_xAl_{1-x} samples quenched from 1000°C , (b) comparison of the development of bulk S parameter and hardness with Al content.

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Slow positron beam with digital Doppler broadening spectrometer and in-situ film deposition by electron evaporation

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A compact magnetically guided continuous variable energy slow positron beam was built at the Charles University, Prague. A ^{22}Na radioisotope with activity of 1.85 GBq (iThemba LABS) is used as a source of fast positrons. Transmission geometry positron moderator consists of a W foil with thickness of 9 μm attached directly to Ti window of the ^{22}Na capsule and followed by a set of four W meshes kept at negative potential gradually decreasing from 0 down to -12 V. Slow positrons are separated by bending of the beam in the magnetic field. Moderated slow positrons can be accelerated up to 30 keV using an electrostatic accelerator. The beam is designed for defect studies of thin films. It is equipped with a chamber for in-situ preparation of films by two electron evaporators (Tectra). Films prepared in the deposition chamber can be transferred to the sample chamber for positron annihilation measurement and back without breaking of vacuum. It enables step-by-step characterization of thin films during growth. Doppler broadening of annihilation photopeak is measured using two high purity Ge detectors with energy resolution of 1.2 keV at 511 keV. Detectors are located in face-to-face geometry perpendicular to the positron beam and can work either independently or in coincidence. Detector signals are worked out using a digital setup [1].

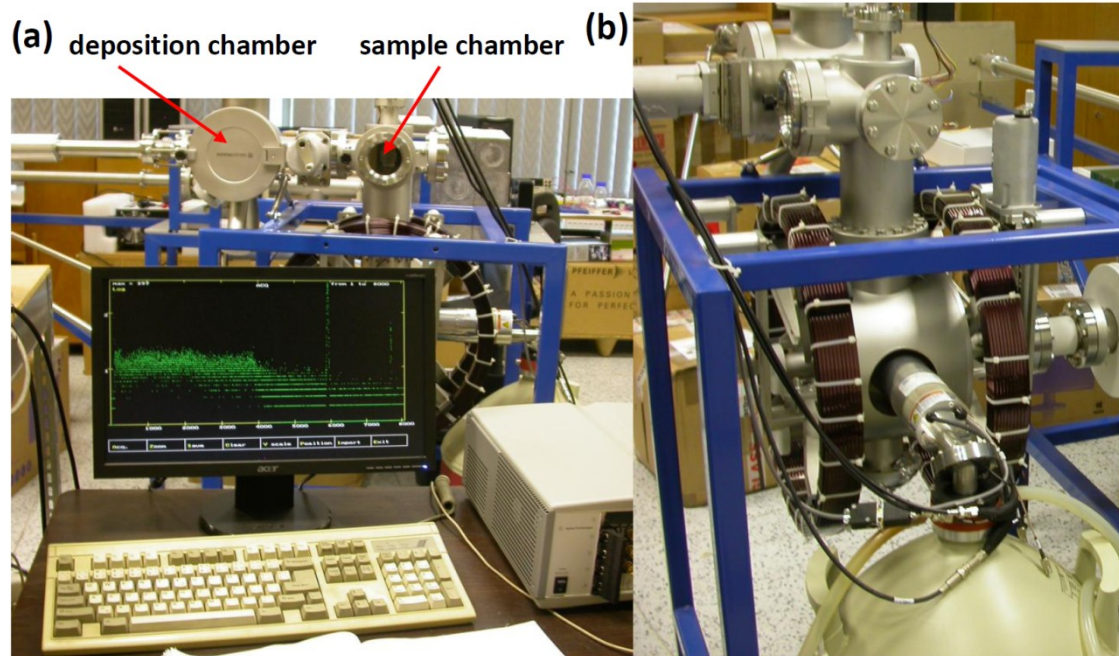


Figure 1 (a) A front view of the slow positron beam, (b) detail of the sample chamber.

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Surface characterization of Si single crystals modified by laser irradiation

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Preamorphization implantation of Si wafer by Si⁺ ions is commonly used in ultrashallow junction formation in order to achieve high dopant activation level and to prevent dopant channeling. A drawback is that implantation leaves a damage band, rich in Si-interstitials. During the post-implantation activation annealing process, Si-interstitials agglomerate into extended defects and evolve via the Ostwald ripening mechanism. These defects are responsible for dopant diffusion and activation anomalies as well as junction leakage. High power laser annealing is a promising alternative for production of a highly activated, ultrashallow, and boxlike junction profile. High fluence excimer laser irradiation melts the surface of the substrate and the melted surface layer subsequently undergoes a liquid phase epitaxy re-growth. However recrystallization of the melted layer may leave undesired point defects beyond the liquid/solid interface. To check this possibility variable energy positron annihilation spectroscopy (VEPAS) was employed to characterize microstructure of sub-surface region of Si single crystals re-grown after surface melting by high power laser treatment. Virgin Si (001) crystal was compared with crystals subjected to laser irradiation with increasing number of laser pulses and with laser power varied in the range from 0.4 to 0.75 J/cm².

From VEPAS measurements one can conclude that Si crystals contain a sub-surface region consisting of a mixture of crystalline and amorphous SiO₂ and also crystalline Si. Laser-induced melting and re-growth cause an increase of crystallinity in the sub-surface region. Thickness of the modified layer corresponds well with the expected depth of the melted region (60 nm). No significant enhancement in the concentration of open volume defects was detected at the interface between the re-grown sub-surface region and Si bulk.

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Positron-impact excitation of the \hat{A}^1B_1 electronic state of water

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We report integral cross sections for positron-impact excitation of the \hat{A}^1B_1 electronic state of water. This is an important channel for the production of radical, as well as for understanding the origin of the atmospheric effects. The idea of using positrons as a tool for scanning the human body in order to identify tumors and other kinds of anomalies represent a important study. Recently we have presented differents applications of the scaling Born positron (SBP) approach and the integral cross sections (ICS) demonstrated the ability of the method [1]. The scaling Born positron (SBP) approach is described as [1]

$$\sigma_{\text{SBP}} = \left\{ \left(\frac{f_{\text{accur}}}{f_{\text{Born}}} \right) \left(\frac{E_0}{[E_0 + E_{\text{ps}} + E_{\text{exc}}]} \right) \right\} \cdot \sigma_{\text{Born}} \quad (1)$$

where E_0 is the incident positron energy, f_{accur} is an accurate dipole value from experiments or from accurate wavefunctions, and f_{Born} is the dipole value from the same wavefunctions used to calculate the unscaled Born cross section (σ_{Born}). E_{ps} represent the positronium energy, and E_{exc} excitation energy. In Fig.1 we present integral cross sections for H_2O using the SBP approach.

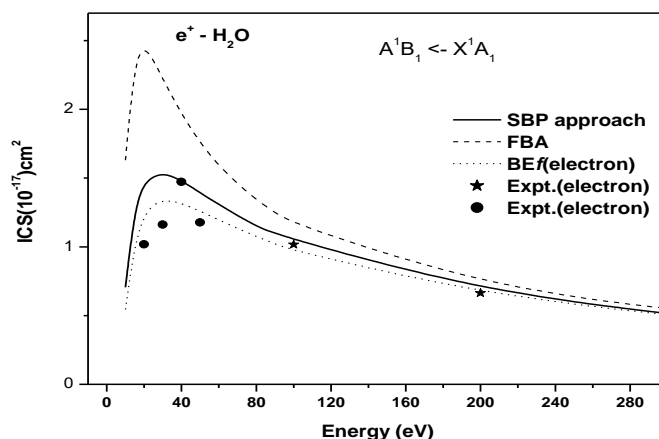


Figure.1 Integral cross sections for $e^+ - \text{H}_2\text{O}$ ($X^1A_1 \rightarrow A^1B_1$) state. Solid line, SBP; dashed line, FBA; dot line, BEf-scaling (electron)[2]; star, and circle black, experimental data (electron)[2].

In the absence of the experimental data, and theoretical studies comparisons are made with analogous electron scattering. We kindly suggest a future experimental verification of the positron scattering cross sections for this molecule.

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Design of picosecond pulsed positron beam for defect characterization

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We present preliminary results of the timing performance of pulsed positron beamline at RCD, BARC as measured using a DC electron gun. The complete beamline consists of – source assembly, ExB filter section, chopper-buncher assembly and the sample chamber [1]. A uniform magnetic field of ~ 80 G is maintained using a series of Helmholtz coils. The picoseconds pulsing of the electron beam is achieved in two steps- (a) chopping and (b) bunching. The chopper consists of three parallel highly transparent tungsten grids, separated from each other by 3 mm. The surface normal of the grids is parallel to the beam direction. The first and third grid are grounded while the middle one is fed a 5W sinusoidal potential of frequency 37.5 MHz[2]. The RF applied to the chopper rides on a DC level adjusted for the beam energy in such a way so as to produce ~ 1 ns pulses. The next stage of picoseconds pulsing is achieved using a 150 MHz quarter wave resonator. It is constructed using two concentric OFHC copper cylinders with their axis parallel to the incident beam. The Q value of the cavity is 750. Operating the buncher cavity at ~ 8 W, we have obtained 280 ps pulses as measured using a fast micro channel plate. Details regarding the RF circuitry, design of various DC and RF components will be presented along with future plans regarding various systems that we intend to study.

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PLRF code for decomposition of positron lifetime spectra

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PLRF is a new code for decomposition of positron lifetime spectra developed in the positron annihilation group at the Charles University, Prague. PLRF code is based on least square fitting of positron lifetime spectra and utilizes a minimization routine MINUIT [1] from the ROOT package [2] developed at CERN. Main features of the PLRF code can be summarized as follows

- (i) possibility to select and combine various strategies of minimization of the χ^2 functional: Monte Carlo, Simplex and gradient algorithm in order to achieve most accurate result of fitting.
- (ii) Multiple positron lifetime spectra can be fitted simultaneously. User can select common parameters which are considered to be the same for all spectra (e.g. positron lifetimes and relative intensities of exponents) and individual parameters which are considered to be different for each spectrum (e.g. position of time zero, parameters of resolution function, etc.)
- (iii) Several models were implemented in the code: independent exponential components, simple trapping model, positron diffusion model, size distribution of clusters. The PLRF code uses physically relevant parameters of the model for fitting and takes into accounts constraints of the parameters within each model. As a consequence user obtains physically meaningful parameters from fitting, e.g. positron trapping rates in case of the simple trapping model, grain size in case of positron diffusion model etc.
- (iv) Positronium contribution is considered as double exponential component consisting of short lived p-Ps and long lived o-Ps component. Ratio of o-Ps and p-Ps contribution can be fixed.

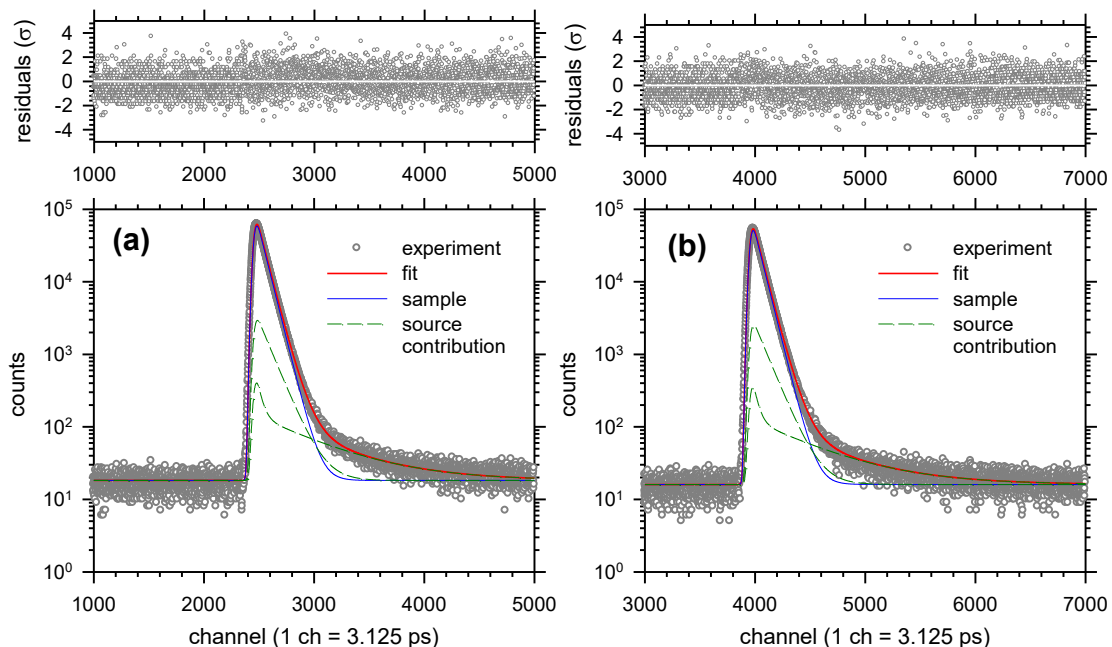


Figure 1 Results of simultaneous fitting of two positron lifetime spectra (a) and (b) of Si (100) single crystal reference sample. Upper panels show residuals in units of one standard deviation.

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