

12th International Workshop on Positron and Positronium Chemistry



Book of Abstracts Programme

Lublin, Poland, August 28 - September 1, 2017

Editors Bożena Zgardzińska, Artur Błażewicz

Organizers



Maria Curie-Skłodowska University, Institute of Physics, Department of Nuclear Methods

Organizing Committee

R. Zaleski (Chair)
B. Zgardzińska (Secretary)
B. Jasińska (Proceedings co-editor)
J. Dryzek (Proceedings co-editor)
M. Budzyński
A. Błażewicz
K. Durak
M. Gorgol
M. Pietrow
Z. Surowiec
M. Wiertel
K. Wysogład

International Scientific Committee

P. K. Pujari (India) Chair
A. Alam (UK)
C. Q. He (China)
T. Hirade (Japan)
Y. C. Jean (USA)
J. Kuriplach (Czech Republic)
Y. Nagashima (Japan)
K. Ratzke (Germany)
D. M. Schrader (USA) Emeritus
F. Selim (USA)
S. V. Stepanov (Russia)
K. Sudarshan (India)
R. Zaleski (Poland)

Honorary Committee

Z. Korczak (Dean of the Faculty of Mathematics, Physics and Computer Science)
S. Michałowski (Rector of Maria Curie-Skłodowska University)
R. Dobrowolski (Vice Rector of UMCS for Science and International Cooperation)
K. Żuk (Mayor of the City of Lublin)
S. Sosnowski (Marshal of the Lubelskie Voivodship)
P. Czarnek (Lubelskie Province Governor)

3|

Honorary patronage



UMCS
WYDZIAŁ MATEMATYKI, FIZYKI
I INFORMATYKI

Zbigniew Korczak, Dean of the Faculty of Mathematics, Physics and Computer Science



UMCS
MARIA CURIE-SKŁODOWSKA UNIVERSITY
IN LUBLIN

Stanisław Michałowski, Rector of Maria Curie-Skłodowska University

**PATRONAT
HONOROWY**



PREZYDENT MIASTA LUBLIN
KRZYSZTOF ŻUK

Krzysztof Żuk, Mayor of the City of Lublin

Honorary patronage



SŁAWOMIR SOSNOWSKI
MARSZAŁEK
WOJEWÓDZTWA LUBELSKIEGO

Sławomir Sosnowski, Marshal of the Lubelskie Voivodship

PATRONAT HONOROWY
WOJEWODA LUBELSKI
PRZEMYSŁAW CZARNEK



Przemysław Czarnek, Lubelskie Province Governor

August 28 - September 01, 2017
Lublin, Poland

Sponsors



IRtech[®]



Contact

Address:

Department of Nuclear Methods
Institute of Physics
Maria Curie-Skłodowska University
Pl. Marii Curie-Skłodowskiej 1
20-031 Lublin

Telephone:

+48 81 537 62 88
+48 81 537 62 86

Internet:

<http://www.ppc12.umcs.pl>
ppc12@umcs.pl

August 28 - September 01, 2017
Lublin, Poland

Oferta firmy IRtech

IRtech, Paweł Warchoń, pawel@irtech.pl

www.irtech.pl

Firma IRtech powstała w 2003 roku. Obecnie nasza oferta obejmuje kilka działów: analizatory substancji chemicznych, generatory gazów, detektory i spektrometry promieniowania alfa, beta i gamma, generatory promieniowania X, systemy analityczne XRF, XRD, SAXS, WAXS, przenośne spektrometry Ramana, FT-IR, GC/MS, NIR, analizatory metali wykorzystujące technikę LIBS i XRF oraz specjalizowane oprogramowanie do zarządzania substancjami chemicznymi.

W dziedzinie detekcji spektrometrii promieniowania nasza oferta jest bardzo bogata. Produktami sztandarowymi są **Spektrometry Promieniowania Gamma z detektorami HPGe**, które produkowane są przez ORTEC. Na szczególną uwagę w tej dziedzinie zasługują spektrometry HPGe chłodzone elektrycznie bez ciekłego azotu oraz nowa seria detektorów semiplanarnych PROFILE z wysoką wydajnością detekcji dla niskich energii i poprawioną energetyczną zdolnością rozdzielczą.

Szczególnej uwadze polecamy zwrócić na nasze **liczniki ciekłoscyntylacyjne Hidex**. Są to zautomatyzowane urządzenia do badań niskotłowych próbek środowiskowych do różnych zastosowań. Wykorzystują innowacyjne rozwiązania technologiczne, takie jak pomiar metodą TDCR (Triple-to-Double-Coincidence-Ratio), Tryb Luminescence Free czy separacja alfa/beta w trybie 2D.

Kryształy scyntylacyjne, detektory CZT oraz inne typy detektorów, analizatory wielokanałowe oraz elektronika(w tym NIM) do obróbki i przetwarzania sygnału jest u nas dostarczana przez producentów gotowych systemów, jak również przez firmy wyspecjalizowane w tej branży, jak na przykład FAST ComTec.

Odchodząc odrobinę od promieniowania, zapraszamy również do zapoznania się z naszymi **generatorami i detektorami promieniowania X do zastosowań w XRF**. Oferujemy systemy laboratoryjne, dowolnie konfigurowalne przez użytkownika jak również gotowe urządzenia podręczne i stacjonarne.

Serdecznie zapraszam do odwiedzenia naszego stoiska i zapoznania się ze szczegółami naszej oferty. Większość urządzeń posiadamy w wersjach demonstracyjnych z możliwością bezpłatnego wypożyczenia.

Pozdrawiam,
Paweł Warchoń

UNI-EXPORT INSTRUMENTS POLSKA

We are offering technical and application support, service and sales of specialized research equipment. We deliver solutions manufactured by leading companies from Europe and the USA but also integrate various systems adapting them to the special requirements and applications.

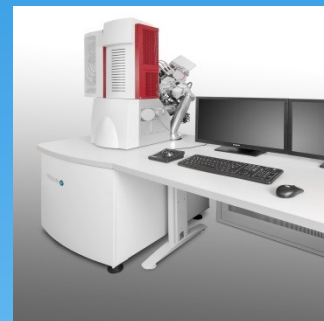
Vacuum technology:

- Pumps and pumping systems: rotary vane, scroll (dry), membrane, turbomolecular, diffusion, ion, cryogenic, high capacity industrial pumps.
- Vacuum gauges and controllers: Pirani, Bayard-Alpert, full range, Baratron etc.
- Vacuum components (hardware) and valves.
- Leak detector based on He detection.
- Mass Flow Controllers – for various flow ranges and applications.
- Mass Spectrometry and RGA, FTIR, pressure and vacuum control, gas and vapor dosing.
- Plasma, microwave and ozon technology.



Scanning electron microscopy:

- Scanning electron microscopes: tungsten, FEG, LaB6.
- SEM based analytical solutions: RAMAN-SEM, FIB-SEM, SIMS-SEM, AFM-SEM.
- Analytical equipment for SEM: EDX, WDX, EBSD.
- Special detectors and accessories: EBIC, CL, cooling/heating, tensile stages.



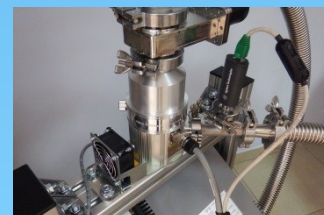
Physico-Chemical Analysis of materials:

- Porosity and surface area measurements, porometry and permeability.
- True and tap density analyzers.
- Gas and vapor sorption analyzers.
- Stability of concentrated emulsions and suspensions, analysis of thin layer formation.



Custom-made solutions and services:

- Vacuum furnaces (laboratory size), special pumping systems
- Thermal coaters for special applications.
- Vacuum gauge controllers designed to work with gauges from various manufacturers.
- Layer thickness detectors for coaters.
- Leak detection stations based on He detection.
- Vacuum gauges and He leak vessels calibration.
- Vacuum pumps repair and rebuilding.



www.uni-export.com.pl



Uni-Export Instruments Polska

Ludwika Kickiego str. 4a lok. 50
04-369 Warsaw, Poland

Tel: +48 22 626 87 86

Fax: +48 22 626 87 85

E-mail: office@uni-export.com.pl

Our partners:



Programme

Monday (28 August)	
09:00	Registration
11:30	Opening session (Chair: R. Zaleski)
	Welcome from K. Żuk (<i>Mayor of the City of Lublin</i>)
	Welcome from R. Dobrowolski (<i>Vice Rector of MCSU</i>)
	A. Alam <i>In memoriam</i>
12:30	Lunch
14:00	Fundamental aspects I (Chair: S. Stepanov)
	G. Consolati <i>Positronium for antihydrogen production: the AEGIS experiment</i>
	J. Van Horn <i>Positron analysis of right- and left-handed alanine single crystals</i>
	K. Fedus <i>Positronium formation in gases and liquids</i>
15:30	Coffee break
16:00	Fundamental aspects II (Chair: G. Consolati)
	S. Stepanov <i>To the positronium formation in liquids</i>
	T. Hirade <i>Ortho-Positronium annihilation in room temperature ionic liquids</i>
	H. Ray <i>Collision between two atoms including Positronium and Muonium</i>
	M. Tachikawa <i>Ab initio theoretical study of the effect of molecular vibrations on the positron-binding to polyatomic molecules</i>
17:30	Welcome party

9|

Tuesday (29 August)		
09:00	Polymers and soft matter I (Chair: F. Selim)	
	A. Alam	<i>Molecular mobility in glass forming matter – the role of free volume: positron annihilation perspectives for industrial applications</i>
	B. Zgardzińska	<i>A new approach to the presentation of the Positron Annihilation Lifetime Spectroscopy results</i>
	E. Dryzek	<i>Positron annihilation in highly ordered smectic E phase of 4-hexyl 4' - isothiocyanatobiphenyl (6TCB)</i>
10:30	Coffee break	
11:00	Polymers and soft matter II (Chair: A. Alam)	
	R. Brusa	<i>Description of molecular transport in epoxy-resin and in graphene-epoxy nanocomposite by experimentally determined fractional free volume</i>
	H. Mohamed	<i>Proton conductivity and free volume properties in per-fluorinated sulfonic acid/PTFE copolymer for fuel cell</i>
	T. Kavetsky	<i>Network properties of ureasil-based polymer matrixes for construction of amperometric biosensors as probed by PALS and swelling experiments</i>
	M. Gomaa	<i>Free volume of PVA/SSA proton exchange membrane studied by positron annihilation lifetime spectroscopy</i>
12:30	Lunch	
14:00	Polymers and soft matter III. Surfaces (Chair: H. Mohamed)	
	P. Pujari	<i>Positron spectroscopic studies of polymer nanocomposites: an overview</i>
	J. Bartos	<i>PALS and ESR evidence of the dynamic crossover in the amorphous phase of the crystalline n-alkanes</i>
	T. Tachibana	<i>Comparative study of positron- and electron-stimulated ion desorption from a TiO₂ (110) surface</i>
	I. Mochizuki	<i>Structure determination of TiO₂ crystal surfaces using total-reflection high-energy positron diffraction (TRHEPD)</i>
	M. Gorgol	<i>Aerogel IC3120 under high pressure, obtained by pistons and nitrogen molecules</i>
15:30	Excursion	
18:00	Dinner	
21:00	Concert	

Wednesday (30 August)		
09:00	Porous materials, nanostructured and confined systems I (Chair: M. Butterling)	
	C. He	<i>Positronium in mesopores of silica thin films</i>
	K. Ito	<i>Nanopore structure of siloxane-silica CVD films elucidated by the low-energy AMOC technique with a radioisotope-based pulsed positron beam</i>
	O. Šauša	<i>Free-volume evolution in 1-propanol confined in partially filled regular mesopores of SBA-15 matrix</i>
10:30	Coffee break	
11:00	Porous materials, nanostructured and confined systems II (Chair: M. Fujinami)	
	B. Wang	<i>Progress of positron detection technology in IHEP and applications</i>
	M. Butterling	<i>Investigation of the porous structure of oblique angle deposited thin films with tailored architectures</i>
	M. Liedke	<i>In-situ investigations of the curing process in ultra low-k materials</i>
12:30	A. Attallah	<i>Porosimetry of ultra-low K materials and transformed porous glass-thin layers by Monenergetic Positron Source at ELBE facility</i>
	Lunch	
	Porous materials, nanostructured and confined systems III, Metals (Chair: C. He)	
	M. Fujinami	<i>Pores in highly densified silica glass by positron annihilation spectroscopy</i>
14:00	S. Yoshimoto	<i>Effect of heat treatment on the nanoporosity of silica PECVD films elucidated by the low-energy positron lifetime technique and ellipsometric porosimetry</i>
	J. Cizek	<i>Positronium formation in nanostructured metals</i>
	V. Krsjak	<i>Nucleation and growth of helium-vacancy clusters in ferritic-martensitic steels effect of dpa rate</i>
15:30	Coffee break	
16:00	Metals, alloys, oxides and semiconductors (Chair: J. Cizek)	
	J. Kuriplach	<i>High entropy HfNbTaTiZr alloys: structure stability, short range order and vacancies</i>
	J. Dryzek	<i>Defect range and evolution in swift Xe-ion irradiated pure silver and titanium studied by positron annihilation techniques</i>
	V. Slugen	<i>PAS studies applied for evaluation of neutron and hydrogen treated reactor steels</i>
17:30	L. Dubov	<i>Investigation of near-surface radiation defects in Si and W by means of conventional positron lifetime spectrometer with a ²²Na positron source</i>
	Poster session	

11 |

Thursday (31 August)		
	Experimental and facilities I (Chair: J. Dryzek)	
09:00	I. Makkonen	<i>Combining experiments and theory in positron annihilation techniques: recent advances and future prospects</i>
	K. Michishio	<i>A collimated, energy-tunable positronium beam for the investigation of positronium scattering with surfaces</i>
	S. Niedźwiecki	<i>Studies performed on previous J-PET prototypes</i>
10:30	Coffee break	
	Experimental and facilities II (Chair: T. Hirade)	
11:00	D. Cassidy	<i>Generation of an electrostatically guided Rydberg-Ps beam</i>
	B. O'Rourke	<i>Recent research and current status of the accelerator based slow positron beam facility at AIST</i>
	Y. Kuzuya	<i>Preliminary evaluation of a brightness enhancement system of the KUR slow positron beamline</i>
	M. Silarski	<i>Studies of the discrete symmetries in the decays of positronium with J-PET tomograph</i>
12:30	Lunch	
	Experimental and facilities III. Metals (Chair: J. Kuriplach)	
14:00	B. Jasińska	<i>New porosimetric method based on 3g/2g annihilation. Applications to material science and medical imaging</i>
	W. Egger	<i>The pulsed low energy positron beam system PLEPS: New developments and applications to polymer and membrane layers</i>
	S. Ishibashi	<i>Two-component density functional study of positron-vacancy interaction in metals and semiconductors</i>
	P. Hruska	<i>Hydrogen interaction with vacancies in Ti</i>
	N. Arutyunov	<i>Positron probing of open vacancy volume of a thermally stable phosphorus-vacancy pair in electron-irradiated silicon</i>
15:30	Coffee break	
16:00	Round table discussion (Moderator: P.K. Pujari) <i>Internal and external cooperation of the positron community</i>	
17:00	Short tour of Lublin	
19:30	Banquet	

Friday (1 September)		
09:00	Practical applications (Chair: B. Jasińska)	
	P. Moskal	<i>Potential of the J-PET tomograph for multi-photon medical imaging</i>
	F. Selim	<i>Advanced positron techniques for practical applications: history, current, and future developments</i>
	G. Korcyl	<i>Online processing of tomographic data</i>
10:30	Coffee break	
11:00	Closing session (Chair: R. Zaleski)	
	F. Selim, J. Dryzek <i>Summary</i>	
12:30	Lunch	

Posters

Fundamental aspects		
P1	M. Pietrow	<i>Application of the theory of excitons to study of the positronium in matter. Optical transition during positronium formation in matter.</i>
P2	J.D. Van Horn	<i>Positron interactions with natural and synthetic chiral quartz crystals in non-z orientations</i>
P3	J. Franz	<i>A database for theoretical positron-molecule cross sections</i>
Polymers and soft matter		
P4	E. Dryzek	<i>Positron annihilation lifetime spectroscopy of ABS objects manufactured by fused deposition modelling</i>
P5	E. Dryzek	<i>Free-volume and mechanical properties of glass fibre reinforced polyamide 6 composites</i>
P6	X. Cao	<i>Extraction of chemical information using positron annihilation spectroscopy in metal-chitosan complex</i>
P7	P. Fang	<i>Study on the surface microstructure of the aged silicone rubber composite insulators by PALS</i>
P8	O. Melikhova	<i>Thermal development of free volumes in Nafion membrane</i>
P9	H. Mohamed	<i>Microstructure characterization of Nafion HP JP as a proton exchange membrane for fuel cell: positron annihilation study</i>
P10	M. Nippa	<i>Free volume in the strained rubber with carbon black filler by positron annihilation spectroscopy</i>
P11	V. Shantarovich	<i>Positron Annihilation and Nanoporosity of Polymeric Membranes and Sorbents</i>
P12	H. Švajdlenková	<i>External probing characterization in relation to relaxation dynamics: cis-1,4-poly(isoprene)</i>
P13	P. Pujari	<i>Free volume characteristics and thermal properties of thin layers of poly vinyl acetate (PVAc) adsorbed on fumed Silica</i>
Porous materials, nanostructured and confined systems		
P14	P. Pujari	<i>Phase transition behaviour of water confined in titania mesopores</i>
P15	K. Čechová	<i>The combined free-volume and thermal response study of the low hydrated Ca-Montmorillonite</i>
P16	M. Gorgol	<i>Controlled porosity of MCM-41 obtained by partial blocking of pores by silicon oil</i>
P17	A. Lider	<i>Positron spectroscopy of nanodiamonds after hydrogen treatment</i>
P18	I. Prochazka	<i>Positronium probing of pores in zirconia nanopowders</i>
P19	N. Sakata	<i>Pores in various kinds of zeolites by positron annihilation spectroscopy</i>
P20	A. Sienkiewicz	<i>Porosity of silica monoliths with tailored mesopores of ink-bottle shape determined by nitrogen adsorption and positron annihilation lifetime spectroscopy</i>
P21	G. Tanzi	<i>A two-particle model for Positronium confined in sub-nanometric cavities</i>
Experimental and facilities		

P22	Y. Akmalova	<i>Evaluation of e⁺ implantation profile for ²²Na positron source</i>
P23	D. Dinescu	<i>Simulations on reducing the influence of backscattered slow positrons on lifetime measurements</i>
P24	K. Dulski	<i>Positronium lifetime measurement using J-PET Detector</i>
P25	N. G. Sharma	<i>Reconstruction of hit-time and hit-position of annihilation quanta in J-PET detector using synchronized model signals</i>
P26	T. Hyodo	<i>Surface Studies at SPF, KEK: Positron Diffraction and Positronium TOF</i>
P27	R. Krause-Rehberg	<i>Improvements in the Production of ²²Na Positron Sources at iThemba LABS</i>
P28	R. Laptev	<i>The semi-digital spectrometric system for positron spectroscopy</i>
P29	B. O'Rourke	<i>Development of sample holders with thin SiN windows for PALS measurement of liquid samples</i>
P30	M. Pawlik-Niedźwiecka	<i>J-PET detector NEMA spatial resolution studies</i>
P31	M. Saro	<i>Optimization of positron-lifetime measurement geometry based on Geant4 simulations</i>
P32	S. Sharma	<i>Time over Threshold (TOT) as a measure of Energy deposition by gamma quanta in plastic scintillator used in J-PET</i>
P33	Shivani	<i>Measurement of gamma quantum interaction point in plastic scintillators with WLS strips</i>
P34	M. Skurzok	<i>J-PET Time Calibration</i>
P35	F.A. Selim	<i>Developing new routine for processing two-dimensional coincidence Doppler energy spectra</i>
Metals, alloys, oxides and semiconductors		
P36	T. Brodziansky	<i>Effect of the initial microstructure on defect evolution in neutron irradiated Fe-Cr-C alloys</i>
P37	K. Durak	<i>Positron annihilation in magnetite nanopowders prepared by coprecipitation method</i>
P38	A. Nozaki	<i>Dominant defects in hydrogen-embrittled iron detected by positron annihilation spectroscopy</i>
P39	M. Sarnek	<i>Estimate the crystallite size for nanocrystalline AISI 316L stainless steel obtained by hydrostatic extrusion method using slow positron beam.</i>
P40	M. Wiertel	<i>Impact of impulse shot peening parameters on properties of stainless steel surface</i>
Practical applications		
P41	E. Kubicz	<i>Cardiac myxoma studies with Positron Annihilation Lifetime Spectroscopy</i>
P42	M. Mohammed	<i>Study the linear polarization of the positron and positronium by using the J-PET detector</i>
P43	K. Wysogład	<i>Human tissue investigations using PALS technique - free radicals influence</i>

Abstracts

oral presentations

Positronium for antihydrogen production in the AEGIS experiment

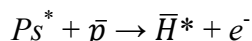
G. Consolati, on behalf of the AEGIS collaboration

*Department of Aerospace Science and Technology, Politecnico di Milano
Piazza Leonardo da Vinci, 32 – 20133 – Milano, Italy*

e-mail: giovanni.consolati@polimi.it

The primary goal of the AEGIS collaboration (Antihydrogen Experiment: Gravity, Interferometry, Spectroscopy) is to measure for the first time precisely the gravitational acceleration of antihydrogen, \bar{H} , a fundamental issue of contemporary physics, using a beam of antiatoms. Indeed, although indirect arguments have been raised against a different acceleration of antimatter with respect to matter, nevertheless some attempts to formulate quantum theories of gravity, or to unify gravity with the other forces consider the possibility of a non-identical gravitational interaction between matter and antimatter.

We plan to generate \bar{H} through a charge-exchange reaction:



between excited Ps and antiprotons coming from the Antiproton Decelerator facility at CERN. This reaction offers the advantage to produce sufficiently cold antihydrogen to make feasible a measurement of gravitational acceleration with reasonable uncertainty (of the order of 1%). Since the cross section of the above reaction increases with n^4 , n being the principal quantum number of Ps, it is essential to generate Ps in a highly excited (Rydberg) state. This will occur by means of two laser excitations of Ps emitted from a nanoporous silica target: a first UV laser (at 205 nm) will bring Ps from the ground to the $n = 3$ state; a second laser pulse (tunable in the range 1650-1700 nm) will excite Ps to the final state. We recently demonstrated both steps of this process [1].

The present paper gives an overview of the AEGIS experiment, describes its current status and discusses how its first goal is thought to be achieved.

[1] S. Aghion et al. (AEGIS collaboration), *Phys. Rev.* **A94**, 012507 (2016)

O2 | **Positron analysis of right- and left-handed alanine single crystals**J.D. Van Horn^{1,*}, B. Eren², F. Wu¹, E. Eren² and Y.C. Jean¹¹*Department of Chemistry, University of Missouri-Kansas City, 5110 Rockhill Rd., Kansas City, Missouri 64110 USA*²*Department of Chemistry, Faculty of Science and Arts, Bilecik Şeyh Edebali University 11210 Bilecik, Turkey*

*email: vanhornj@umkc.edu

Studies of the interaction of polarized light or particles (including electrons, e^- , or positrons, e^+) with asymmetric forms of matter has been of interest to scientists since the discovery of chirality and of particle physics. Researchers have been interested in e^+ interactions with chiral molecules for decades, but with indecisive results [e.g. 1, 2]. After reviewing the field, we speculated that the e^+ or positronium (Ps) might interact differently with chiral pairs of large enantiomeric single crystals—i.e. LH and RH asymmetric forms—and found significant differences in “free positron” annihilation and intensities in evaluating L and R quartz crystals [3]. To extend this line of research we crystallized large D- and L-alanine crystals and performed PALS measurements using a Na-22 positron source.

Alanine crystals were obtained via slow evaporation of water in a Dewar, or from water/acetone solvent in a temperature-controlled environment (Fig. 1). These methods resulted in small (~ 0.5 cm³) or large (> 1.0 cm³/side) crystals, respectively. Intensity (I_2) results from LH and RH crystals were different in PALS analysis (e.g. Fig. 1, right). Aspects of asymmetric crystals, stereo-recognition, and stereo-selection will be discussed, as well as prior positron experiments with asymmetric forms of matter. The result here may be considered a follow-up study and extension of early work by Garay, *et al.* [4], Rich [5], and others over the years investigating the PAS of D- and L-amino acids.

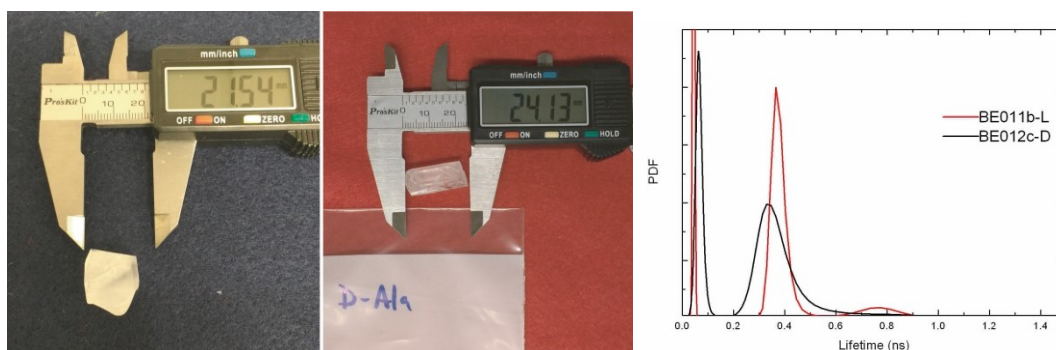


Fig.1. Examples of large L- and D-alanine crystals. MELT analysis of PALS data for small (~ 0.5 cm) L- and D-alanine crystals.

- [1] Y.C. Jean and H.J. Ache. *J. Phys. Chem.* 81, 1157 (1976)
- [2] L. Chiari, A. Zecca, S. Girardi, A. Defant, F. Wang, X.G. Ma, M. V. Perkins and M.J. Brunger, *Phys. Rev. A*, 85, 052711 (2012)
- [3] J.D. Van Horn, F. Wu, G. Corsiglia and Y.C. Jean, *Defect. Diffus. Forum.* 373, 221 (2016)
- [4] A.S. Garay, L. Keszthekyi, I. Demeter and P. Hrasko, *Nature* 250, 332 (1974)
- [5] A. Rich, *Nature* 264, 482 (1976)

Positronium formation in gases and liquids

K. Fedus, A. Karbowski, G. Karwasz

*Institute of Physics, Nicolaus Copernicus University,
Grudziadzka 5, 87-100 Toruń, Poland*

*email: kamil@fizyka.umk.pl

Development of medical imaging techniques based on positron annihilation [1] triggered a renewed interest in fundamental studies of positron scattering by organic molecules. Such studies require the complementary information from different research fields. On the one hand an accurate experimental characterization of positron behavior in condensed matter is necessary in order to grasp a main features of positron collective interaction with dense molecular environment. On the other hand the knowledge about the basic interactions occurring on molecular scale over a wide energy range is indispensable for modeling purposes. In particular the scattering cross section, measured in the gas-phase conditions, are required as inputs for modeling codes [2]. In this context, experimental and theoretical total positron scattering and positronium formation cross sections from organic molecules are necessary.

The aim of this work is twofold. Firstly, we re-discuss main problems related with the determination of positron scattering and positronium formation cross-sections for gas-phase molecules [3]. Examples of benzene, cyclohexane and methanol are given. Some semi-empirical analysis of scattering cross-sections below Ps formation is presented [4]. Secondly, we report the positron lifetime measurements in liquid-phase of these three molecules as a function of both temperature and air content. Air presence changes significantly the value of the third component; surprisingly we observed little influence on the intensity of this component.

[1] N. G. Sharma *et al.*, J. Chem. Pharm. Sci., Special Issue 4, 927 (2016)

[2] F. Blanco *et al.*, J. Phys. B: At. Mol. Opt. Phys. 49, 145001 (2016)

[3] G.P. Karwasz, D. Pliszka, R.S. Brusa, C. Perazzolli, A. Zecca, Acta Phys. Pol. 107, 666 (2005)

[4] K. Fedus, Phys. Scr. 89, 1 (2014)

To the positronium formation in liquids

S.V. Stepanov^{1,2,*}, V.M. Byakov¹⁻³, P.S. Stepanov⁴ and D.S. Zvezhinskiy¹

¹NRC “Kurchatov Institute” – Institute of Theoretical and Experimental Physics,
B.Cheremuskinskaya st., 25. 117218 Moscow Russia

²National Research Nuclear University “MEPhI”, 115409, Moscow, Russia

³D. Mendeleyev University of Chemical Technology of Russia, Miusskaya sq., 9, 125047,
Moscow, Russia

⁴Department of Physics and Astronomy, 104 Overmann Hall, Bowling Green State University,
OH, 43403, USA

*e-mail: stepanov@itep.ru

We describe the e⁺ fate since its injection into a molecular liquid until its annihilation. Several stages are discussed [1-3]:

1) track structure of fast positrons: time and range of ionization slowing down, number of produced ion-electron pairs, thermalization, solvation, chemical interactions between e⁺ and its blob reactants, e⁺ escape from the blob; influence of electric field

2) effect of local heating of the e⁺ blob;

3) positronium formation in liquids. Precursors of the Ps atom (e_{qf}, e_{loc}, e_{solv}). Quasifree Ps state. Can Ps dissociate into e⁺ and e⁻ ?

4) Ps bubble models. Internal energy of e⁺e⁻ pair as a driving force of Ps formation (“non-point” positronium).

5) intratrack diffusion-controlled reactions: Ps oxidation by chemically active radiolytic products.

[1] S.V. Stepanov, V.M. Byakov, D.S. Zvezhinskiy et al., *Advances in Physical Chemistry*, 2012, Article ID 431962, (2012)

[2] S.V. Stepanov, V.M. Byakov, G. Duplatre, D.S. Zvezhinskiy, P.S. Stepanov, A.G. Zaluzhnyi *Journal of Physics: Conference Series*, 618, 012003, (2015)

[3] S.V. Stepanov, V.M. Byakov, D.S. Zvezhinskiy, G. Duplatre *Defect and Diffusion Forum*, 373, pp.17-22, (2017)

Ortho-Positronium annihilation in room temperature ionic liquidsT. Hirade^{1,2*}¹*Nuclear Science and Engineering Center, Japan Atomic Energy Agency,
Tokai, 319-1195 Japan*²*Institute of Quantum Beam Science, Ibaraki University, 4-12-1 Narusawa, Hitachi, Ibaraki,
316-8511 Japan*

*email: t.hirade@kurenai.waseda.jp

The longest annihilation lifetime component is caused by the pick-off annihilation process of triplet Positronium (Ps) i.e. ortho-Positronium(o-Ps) in insulating materials. Ps creates a bubble in liquids because of negative work function of Ps and localize in it. The size of the bubble is controlled by the balance between zero point energy of Ps and energies of volume and surface of the bubble. Therefore, there is a good correlation between o-Ps pick-off annihilation rates and surface tension for many liquids [1]. Furthermore Tao-Eldrup model gives relation between bubble sizes and o-Ps pick-off annihilation rates in many liquids [2].

The positron annihilation lifetime measurements in RTILs showed very strange results [3]. Finally, positron annihilation age-momentum correlation (AMOC) measurements indicated that it was caused by slow bubble formation in RTILs [4]. Then I discovered the oscillation of o-Ps annihilation rates in room temperature ionic liquids (RTILs) which indicated, probably, the oscillation of the Ps bubble [5, 6]. Stepanov et al. [7] calculated change of the bubble size in many liquids and the oscillation of the bubble was not expected except for a liquid He. It means that the structure of RTILs in nanometer scale is very different from usual liquids. Moreover, o-Ps pick-off annihilation rates seems to be too small for the macroscopic surface tension of RTILs.

I am going to discuss what you can study by the positron annihilation methods for the structure of RTILs in nanometer scale.

This research was partially supported by a Ministry of Education, Culture, Sports, Science and Technology Grant-in-Aid for Scientific Research (C) 16K05026, 2016-2018.

- [1] S. J. Tao, J. Chem. Phys. 56 (1972) 5499
- [2] M. Eldrup, D. Lightbody, and J. N. Sherwood, Chem. Phys., 63 (1981) 51.
- [3] T. Hirade, Materials Science Forum, 607 (2009) 232-234
- [4] T. Hirade, T. Oka, Journal of Physics: Conference Series 443 (2013) 012060
- [5] T. Hirade, JJAP Conf. Proc. (2014) 011003
- [6] T. Hirade, Journal of Physics: Conference Series 618 (2015) 012004
- [7] S. V. Stepanov, M. K. Mikhin, D. S. Zvezhinskii, V. M. Byakov, Radi. Phys. Chem. 76 (2007) 275

Collision between two atoms including Positronium and Muonium

H. Ray^{1,2,3*}¹ Study Center JnganSikha, S-1/407/6, B. P. Township, Kolkata 700094, India² Department of Physics, New Alipore College, Kolkata 700053, India³ Science Department, National Institute of TTT and Research, Kolkata 700106, India

*email: hasi_ray@yahoo.com

Recently Ray [1-5] has solved a four-body Coulomb problem exactly in the center of mass frame and introduced two new codes: the SEM and the MSEM to study cold-atomic collision following a coupled-channel methodology. The SEM include the non-adiabatic short-range effect due to electron exchange. The MSEM include the effect due to long-range van der Waals interaction in addition to the short-range non-adiabatic effect. Both these effects dominate at cold energies. The SEM code is applied to study the Ps-H, Ps-Ps, Ps-Mu, Ps-D, Ps-T, Mu-Mu, Mu-H, Mu-D, Mu-T, H-H, H-D, H-T, D-D, D-T and T-T systems. Here Ps, Mu, H, D, T symbolize the Positronium, Muonium, Hydrogen, Deuterium and Tritium respectively. The MSEM code was used to study the variation of scattering length with the variation of the strength of attractive long-range van der Waals interaction controlling the minimum interatomic distances (R_0) as $2a_0$, $3a_0$, $4a_0$, $5a_0$, $6a_0$, $7a_0$, $8a_0$, $9a_0$, $10a_0$, $11a_0$, $12a_0$, $15a_0$, $20a_0$. The systems studied were Ps-H [1] and H-H [5]. It was found that at larger interatomic distances e.g. at $R_0=20a_0$, the MSEM and SEM data nearly coincide. In the present study, I reinvestigate thoroughly both the codes and reproduced exactly the same data to strengthen the earlier findings. Figures 1 and 2, briefly describe the results.

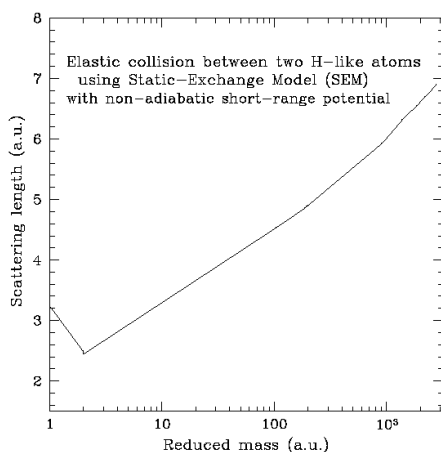


Fig.1. Dependence of scattering length on reduced mass of the system.

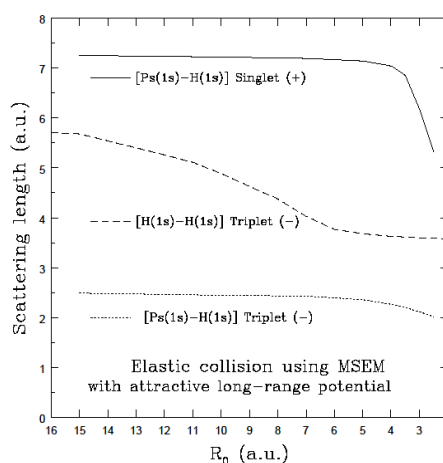


Fig.2. Dependence of scattering length on the strength of van der Waals interaction.

- [1] H. Ray, Pramana J. Phys. 83, 907 (2014).
- [2] H. Ray and R. De, J. Phys. B Conference Series 618, 012008 (2015).
- [3] H. Ray and A. De, J. Phys. B Conference Series 388, 122002 (2012).
- [4] H. Ray, Pramana J. Physics, 86, 1077 (2016).
- [5] H. Ray, Pramana J. Phys. Rapid communication 87, 8 (2016).

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

M. Tachikawa*

*Graduate School of NanoBioScience, Yokohama City University,
22-2, Seto, Kanazawa-ku, Yokohama 236-0027, Japan*

*email: tachi@yokohama-cu.ac.jp

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, are 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 [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 positron affinities, based on *ab initio* multi-component quantum Monte Carlo (QMC) [2] and molecular orbital (MCMO) [3, 4] methods for the electronic and positronic wave functions simultaneously, and the anharmonic vibrational state theory using quantum Monte Carlo (QMC) method [5, 6]. In the case of formaldehyde (CH₂O) 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 drastically enhances the PA value, whereas the excitation of CH₂ 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. Our most accurate prediction of the vibrational averaged PA values at the fundamental and overtone states are 31 and 36 meV, respectively, which strongly supports the conclusion that a positron can bind to formaldehyde [6]. We would like to also show some application of the positron-binding to large BIOMolecules such as amino acids [7] and DNA species [8].

References

- [1] G. F. Gribakin, J. A. Young, and C. M. Surko, *Rev. Mod. Phys.* **82**, 2557 (2010), J. R. Danielson, J. J. Gosselin, and C. M. Surko, *Phys. Rev. Lett.* **104**, 233201 (2010), J. R. Danielson, A. C. L. Jones, M. R. Natisin, and C. M. Surko, *Phys. Rev. Lett.* **109**, 113201 (2012).
- [2] Y. Kita, R. Maezono, MT, M. Towler, R. J. Needs, *J. Chem. Phys.* **131**, 134310 (2009), **135**, 054108 (2011).
- [3] MT, R. J. Buenker, M. Kimura, *J. Chem. Phys.* **119**, 5005 (2003).
- [4] MT, Y. Kita, R. J. Buenker, *Phys. Chem. Chem. Phys.* **13**, 2701 (2011), *New J. Phys.* **14**, 035004 (2012).
- [5] K. Koyanagi, Y. Takeda, T. Oyamada, Y. Kita, MT, *Phys. Chem. Chem. Phys.* **15**, 16208 (2013), Y. Kita and MT, *Eur. Phys. J. D* **68**, 116 (2014).
- [6] Y. Yamada, YK, MT, *Phys. Rev. A* **89**, 062711 (2014).
- [6] K. Koyanagi, Y. Kita, and MT, *Eur. Phys. J. D*, **66**, 121 (7pages) (2012), Y. Oba and MT, *Int. J. Quant. Chem.* **114**, 1146-1149 (2014).
- [7] K. Koyanagi, Y. Kita, Y. Shigeta, and MT, *ChemPhysChem (Communication)*, **14**, 3458-3462 (2013).

O8 | **Molecular mobility in glass forming matter – the role of free volume: positron annihilation perspectives for industrial applications**

M. A. Alam^{1*}, G. Badolato-Boenisch², P. Beavis³, A. Coveney¹, D. Hughes¹, J. Lewicki⁴, C. Schaefer² and J. Ubbink^{1,5}

¹*H.H. Wills Physics Laboratory, Univ. of Bristol, Tyndall Ave. Bristol BS8 1TL, UK*

²*DSM Nutritional Products Ltd, Wurmisweg 576, CH-4303 Kaiseraugst, Switzerland*

³*AWE, Aldermaston, Reading, RG7 4PR, UK*

⁴*Lawrence Livermore National Lab., Livermore, CA 94550, USA*

⁵*Food Sc. and Nutrition Dept. California Polytech. State Univ. San Luis, CA 9340, USA*

*email: m.a.alam@bristol.ac.uk

Positron Annihilation based experimental techniques, in particular Lifetime Spectroscopy (PALS) is now a unique, versatile and well-established tool for direct evaluations of the local free volumes and associated physical/chemical phenomena in glassy matrices. The local free volume in glass forming matter, consists of a large number of sub-nanometre sized open volume “elements” (often referred to as “holes”) which naturally exist in these materials due to their irregular molecular packing, density fluctuations and topological constraints [1]. The free volume plays a crucial role on molecular mobility and, thus, on related material properties such as diffusion (self or of ‘ingressing molecules’), the glass transition, mechanical strength and a diverse range of other physical behaviour [2]. Over the past decade, we and many other groups have successfully used PALS, in conjunction with more traditional experimental techniques, to study a range of practical implications of the free volume in polymers and related materials for a wide range of industrial applications.

So far, much of the studies have concentrated on bulk properties using radio-isotope positron sources with considerable success. This will form the main basis of this presentation. However, there is ample room to investigate practical applications involving ‘glass transition’ behaviour in confined geometries such as in thin films, porous media or at surfaces and interfaces which will be touched upon in the presentation. We propose to give a ‘selective’ overview of the above activities in recent years. The talk would concentrate on relevant work of the Bristol positron group in this area [3] along with a brief sketch of other similar activities within the positron community. We shall also speculate about avenues of possible future direction(s).

[1] Y. C. Jean, P. E. Mallon and D. E. Schrader *Principles and Applications of Positron and Positronium Chemistry*, World Scientific (2003).

[2] G. Dlubek, in *Polymer Physics: From Suspensions to Nanocomposites and Beyond*, eds. L.A. Utracki and A.M. Jamieson, John Wiley & Sons (2011)

[3] Bristol Group and collaborators: *Biomacromolecules*, 11, 3237 (2010), *New J. Phys.* 14, 035016 (2012), *Energy & Env. Sci.* 5, 8359 (2012), *Polymer*, 55, 6827 (2014), *New J. Phys.* 16, 103030 (2014), *Carbohydrate Pol.*, 102, 566 (2014), *Biomacromolecules*, 16, 1784 (2015), *Food Hydrocolloids*, 58, 75 (2016), *Food Hydrocolloids*, 58, 316 (2016).

O9 | A new approach to the presentation of the Positron Annihilation Lifetime Spectroscopy results

B. Zgardzińska^{1,*}, K. Standzikowski²

¹*Institute of Physics, Maria Curie Skłodowska University, 20-031 Lublin, Poland*

²*Department of Geoecology and Palaeogeography, Maria Curie-Skłodowska University
Lublin, al. Kraśnicka 2cd, 20-718 Lublin, Poland*

*email: bozena.zgardzinska@poczta.umcs.lublin.pl

The PALS technique (Positron Annihilation Lifetime Spectroscopy) is used to determine the phase transitions points in the matter (organics, polymers, glasses). Until now it was generally accepted to present and analysis the changes of the spectra parameters (especially the lifetime and the intensity of o-Ps) as a function of external factors, e.g. temperature and pressure, which is correlated with the phase transitions occurring in the medium. We propose a different, new approach in the presentation and analysis of the results, which – as we show – brings important information about the nature of the phase transitions and gives new look at the distinguishing of phases in organic compounds. We have found a general trends in o-Ps parameters closely related to the crystallographic structure in groups of compounds based on the figure in the coordinates (I_3 , τ_3). We propose to include (join) such a presentation of the results to the standard demonstrated in the papers dependencies.

O10 | **Positron annihilation in highly ordered smectic E phase of 4-hexyl 4' – isothiocyantobiphenyl (6TCB)**

E. Dryzek^{1,*}, E. Juszyńska¹, R. Zaleski², B. Jasińska² and M. Ramos Silva³

¹*Institute of Nuclear Physics Polish Academy of Sciences, PL-31342 Kraków, Poland*

²*Institute of Physics, Marii Curie- Skłodowska University, Pl. M. Curie – Skłodowskiej 1, 20-031 Lublin, Poland*

³*CQC, Department of Chemistry, University of Coimbra, Coimbra, Portugal*

*email: ewa.dryzek@ifj.edu.pl

Positron annihilation lifetime spectroscopy (PALS) has been employed for characterization of the local structure in molecular substances such as polymers or liquid crystals. For many liquid crystal forming materials the sensitivity of the positron annihilation parameters to phase transformations has been demonstrated. In such materials not only local microstructure but also molecular dynamics can influence the Ps lifetime and its intensity as it was demonstrated in our studies of supercooled smectic E (SmE) phase of 4TCB [1,2]. The obtained value of *o*-Ps for 4TCB can be explained by formation of Ps bubbles due to a liquid-like state of the butyl chains molecules in the SmE phase and the lamellar structure with nano-segregation of alkyl chains and other parts of molecules proposed by Saito et al. [3].

The present studies were performed for the other member of the nTCB homologous series, i.e. 6TCB. The obtained temperature dependencies of the *o*-Ps lifetime and its intensity for the supercooled SmE phase indicate two processes taking place during heating of the sample. Softening of the glass phase and cold crystallization occurring simultaneously can pose a difficult problem for PALS data analysis and interpretation. The two processes cannot be resolved in PALS measurements as it was in the case of 4TCB thanks to difficult and lengthy crystallization of the latter. The proposed explanation of the obtained dependencies may shed light on the results of previous PALS studies of supercooled liquid crystals reported in the literature.

[1] E. Dryzek, E. Juszyńska, R. Zaleski, B. Jasińska, M. Gorgol, M. Massalska-Arodź, Phys. Rev. E, **88**, 022504 (2013)

[2] E. Dryzek, E. Juszyńska, Phys. Rev. E **93** (2016) 022705

[3] K. Saito, T. Miyazawa, A. Fujiwara, M. Hishida, H. Saitoh, M. Massalska-Arodź, Y. Yamamura J Chem Phys **139**, 114902 (2013)

O11 | **Description of molecular transport in epoxy-resin and in graphene-epoxy nanocomposite by experimentally determined fractional free volume**R. S. Brusa^{1,*}, R. Checchetto² and D. Roilo²¹ TIFPA-INFN and University of Trento-Department of Physics, Via Sommarive 14, 38123 Povo, Trento, Italy² University of Trento-Department of Physics, Via Sommarive 14, 38123 Povo, Trento, Italy

*email: brusa @science.unitn.it

Molecular transport properties of light gases in epoxy-resins membranes with different cross linking density and in epoxy-resins modified with dispersed Few Layer Graphene (FLG) nano-platelets will be discussed in the framework of the free volume theory [1-5].

Four types of resins were prepared by altering their cross-linking densities and hence their glass transition temperature. Nanocomposite membranes were prepared with 1, 5, 7.5, 10 wt.% FLG filler content.

PALS measurements were performed with a fast-fast lifetime set-up with a time resolution of 260 ps. The transport of light gases (H₂, N₂, CO₂) was studied by gas phase permeation techniques up to 350 K temperature.

X-ray diffraction, vibrational spectroscopy and scanning electron microscopy analysis were also performed to characterize the structure of the pure and nanocomposite membranes.

Gas phase permeation measurements show that the transport through the pure membranes obeys to the solution diffusion mechanism. Decreasing the cross-linking density both the permeability and the CO₂/N₂ selectivity increases. [1,2]

The fractional free volume $f_h(T)$ and its evolution with the temperature was experimentally evaluated by measuring the hole dimensions by PALS, the thermal expansion coefficient of the hole free volume and the volumetric thermal expansion coefficient.

The gas diffusion constant of CO₂ and the permeability of H₂, N₂ and CO₂ as a function of temperature was reproduced with the free volume theory and using as input parameter the experimentally evaluated fractional free volume $f_h(T)$ data [3,4].

In the nanocomposite membranes dispersion of filler showed a barrier effect on gas transport. PALS analysis indicated that the free volume structure did not change but the fractional free volume decreased with increasing the filler content. Thanks this finding the change of gas transport properties due to fillers was explained and modelled by the formation of a rigidified polymeric region around fillers. [5]

[1] P. N. Patil, D. Roilo, R.S. Brusa, A. Miotello, R. Checchetto, , *Polymer* **58**, 130 (2015)

[2] P. N. Patil, R. Checchetto, R. Ferragut, S. Aghion, A. Miotello, R.S. Brusa, *J. Phys. Conf. Ser.* **618**, 012036 (2015)

[3] P. N. Patil, D. Roilo, R.S. Brusa, A. Miotello, S. Aghion, R. Ferragut and R. Checchetto, *Phys. Chem. Phys.* **18**, 3817 (2016)

[4] D. Roilo, P. N. Patil, R.S. Brusa, A. Miotello and R. Checchetto *Polymer* **113**, 147 (2017)

[5] D. Roilo, P. N. Patil, R.S. Brusa, A. Miotello, S. Aghion, R. Ferragut and R. Checchetto *Polymer* **121**, 17 (2017)

O12 | **Proton conductivity and free volume properties in per-fluorinated sulfonic acid/PTFE copolymer for fuel cell**

Hamdy F.M. Mohamed^{*1,2}, E.E. Abdel-Hady¹ and M.O. Abdel-Hamed¹

¹*Physics Department, Faculty of Science, Minia University, P.O. Box 61519 Minia, Egypt*

²*Renewable Energy Science & Engineering Department, Faculty of Postgraduate Studies for Advanced Science (PSAS), Beni-Suef University, P.O. Box 62511 Beni-Suef, Egypt*

*email: hamdyfm@gmail.com

The mechanism of proton conductivity in per-fluorinated sulfonic acid/PTFE copolymer Fumapem® membranes for polymer electrolyte fuel cells has been investigated. Three different samples, Fumapem® F-950, F-1050 and F-14100 membranes with ion exchange capacity (IEC) = 1.05, 0.95 and 0.71 meq/g, respectively were used after drying. Free volume was quantified using the positron annihilation lifetime (PAL) technique while the proton conductivities (σ) were measured using LCR Bridge as function of temperature. It was found that as the ion exchange capacity increases, the proton conductivity increases and the free volume expands. Temperature dependences of free volume and also proton conductivity reflect the glass transition temperature of the membrane. Good linear correlations between the reciprocal of the *o*-Ps hole volume size ($1/V_{o-Ps}$) and $\text{Log } (\sigma) + \Delta E_a/2.303 \text{ KT}$, [where ΔE_a is the activation energy, K is the Boltzmann constant and T is the absolute temperature] at different temperature indicate that the ionic motion in dry Fumapem® is governed by the free volume. A good linear correlation between the critical hole size γV_i^* and the ionic exchange capacity was achieved.

O13 | **Network properties of ureasil-based polymer matrixes for construction of amperometric biosensors as probed by PALS and swelling experiments**

T. Kavetsky^{1,2*}, O. Šauša³, K. Čechová³, H. Švajdlenková⁴, I. Matko³, T. Petkova⁵, V. Boev⁵, V. Ilcheva⁵, O. Smutok⁶, Y. Kukhazh² and M. Gonchar⁶

¹*The John Paul II Catholic University of Lublin, Al. Raclawickie 14, 20-950 Lublin, Poland*

²*Drohobych Ivan Franko State Pedagogical University, I. Franko Str. 24, 82100 Drohobych, Ukraine*

³*Institute of Physics, Slovak Academy of Sciences, Dúbravská cesta 9, 845 11 Bratislava, Slovak Republic*

⁴*Polymer Institute, Slovak Academy of Sciences, Dúbravská cesta 9, 845 41 Bratislava, Slovak Republic*

⁵*Institute of Electrochemistry and Energy Systems, Bulgarian Academy of Sciences, Acad. G. Bonchev Str. Bl.10, 1113 Sofia, Bulgaria*

⁶*Institute of Cell Biology, National Academy of Sciences of Ukraine, Drahomanov Str. 14/16, 79005 Lviv, Ukraine*

*email: kavetsky@yaho.com

Recently, innovative amperometric biosensors for monitoring the level of wastewater pollution have been constructed [1] on the surface of the gold planar electrodes C220AT “DropSens” by using the organic-inorganic ureasil-based composites as host polymer matrixes and immobilized commercial laccase from *Trametes versicolor*. It has been found that the biosensor based on the ureasil-chalcogenide glass composite was characterized by very high sensitivity to be 38.3 times higher in compare with pure ureasil. On the other hand, application of the ureasil-chalcogenide glass composite with incorporated silver nanoparticles synthesized by high-dose 30 keV Ag⁺ ion implantation results in decreasing the biosensor sensitivity up to 2390 times. Therefore, knowing the properties of the microstructure of such materials is important in terms of optimizing the regulated properties of the biosensors.

In the present work, the free-volume and swelling properties of various samples of pure ureasil and ureasil-chalcogenide glass composite were studied. Using positron annihilation lifetime spectroscopy (PALS), temperature dependencies of the *ortho*-positronium (*o*-Ps) lifetimes and their relative intensities were measured to estimate the evolution of microstructural free-volume. Glass transition temperatures and expansion coefficients of microscopical free-volume were determined. Differences in network behavior for older samples (aging effect) and the effect of chalcogenide (As₂S₃) particles on the free volume of ureasil network were observed. Swelling experiments using water and ethyl alcohol showed that the structure of the older sample network had less swelling ability for pure ureasil as well as composite. This suggests that the one of factors influencing swelling is the change of the basic ureasil network due to aging.

It is supposed that the network properties obtained by PALS and swelling experiments could be very helpful to understand better the bio-functionality of the constructed biosensor based on the ureasil-chalcogenide glass composite [1].

[1] T. Kavetsky, O. Smutok, M. Gonchar, O. Demkiv, H. Klepach, Y. Kukhazh, O. Šauša, T. Petkova, V. Boev, V. Ilcheva, P. Petkov and A.L. Stepanov, *Journal of Applied Polymer Science* **134**, 45278 (2017)

O14 | **Free volume of PVA/SSA proton exchange membrane studied by positron annihilation lifetime spectroscopy**

Mahmoud M. Gomaa^{1, 2, *}, Christoph Hugenschmidt¹, M.O. Abdel-Hamed²,
E. E. Abdel-Hady² and Hamdy F. M. Mohamed²

¹*FRM II and Physik-Department, Technische Universität München, 85748 Garching, Germany*

²*Physics Department, Faculty of Science, Minia University, P.O. Box 61519 Minia, Egypt.*

*email: mahmoud_gomaa19@mu.edu.eg

Humidity control and water management in polymer electrolyte fuel cells (PEMFC) still remain one of highest importance for increasing the efficiency and development of fuel cell stacks. In this study, poly(vinyl alcohol) was crosslinked using 5-30 wt% sulfosuccinic acid (SSA) by a solution casting method and additional thermally crosslinked at 100°C. Ion exchange capacity (IEC) of the membranes were in the range of 1.093-2.064 mmole/g. The thermal stability of PVA/SSA solid membranes was studied by thermogravimetric analysis (TGA), and it was found that the thermal stability of the membranes improved with increasing SSA content. Positron annihilation lifetime spectroscopy (PALS) was used in order to study the change of total free volume and for distinguishing the void size distribution at different humidity. It was found that the free volume and the water uptake is strongly correlated. The mean void size, however, was found to be related to the mechanical strength of the membranes. In addition, it was found that up to a relative of 30 RH % the ortho positronium lifetime doesn't change significantly whereas it increases strongly with increasing humidity of more than 30RH% as shown in figure 1. Moreover we observe that the conductivity was found in the range 0.216–1.56 mS/cm depending on both the temperature and the SSA concentration.

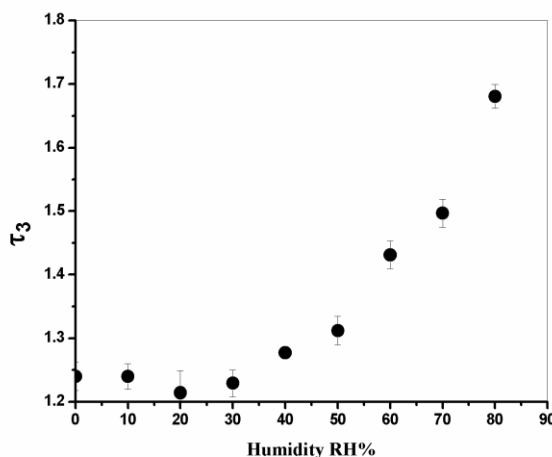


Fig.1. Ortho positronium lifetime τ_3 of PVA with 15% SSA membrane at different humidity.

O15 | **Positron spectroscopic studies of polymer nanocomposites: an overview**

P. K. Pujari*

*Radiochemistry Division, Bhabha Atomic Research Centre, Trombay, Mumbai – 400085,
India*

*email: pujari@barc.gov.in

Polymer nanocomposites (PNCs) are multiphase materials made of polymer matrix reinforced with nanodimensional inorganic fillers [1]. PNCs are shown to have improved mechanical, electrical and thermal properties compared to pure polymers. As a result, PNCs are shown to have increased applications in various industries [2]. The enhancement in the bulk properties are generally correlated to morphology and properties of nanofillers. In recent years, it has been shown that on incorporation of nanofillers in polymer matrices, the molecular level structure of polymer phase is altered. In this regard, formation of an interfacial layer around the nanofillers due to interfacial interaction is well accepted phenomenon in the field of polymer nanocomposites. Investigation of factors responsible for the creation of interfacial layer, structure of interfacial layer as well as its correlations with the bulk physical properties is an active area of research. In last few years, we have used positron annihilation lifetime spectroscopy (PALS) for the investigation of free volume structure in variety of polymer nanocomposites supplemented by other conventional characterization techniques [3-10]. These studies have shown that free volume size, their number density as well as their size distributions are altered in polymer nanocomposites. The observed variations have been explained considering the formation of an interfacial layer. The studies have shown that the free volume characteristics of interfacial layer primarily depend on interfacial interaction between nanofillers and polymer molecules along with the shape and size of nanofillers. The role of interfacial layer characteristics on mechanical and thermal properties has been investigated. An overview of our recent studies on polymer nanocomposites using PALS will be discussed.

- [1] A. C Balazs, T. Emrick and T. P. Russell *Science* 314 1107 (2006).
- [2] L. Z. Guan, Y. J. Wan, L. X. Gong, D. Yan, L. C. Tang, L. B. Wu, J. X. Jiang and G. Q. Lai *J. Mater. Chem. A* 2, 15058 (2014).
- [3] S. K. Sharma, J. Prakash, K. Sudarshan, P. Maheshwari, D. Sathiamoorthy and P. K. Pujari, *Phys. Chem. Chem. Phys.* 14 10972 (2012).
- [4] S. K. Sharma, J. Bahadur, P. N. Patil, P. Maheshwari, S. Mukherjee, S. Mazumder and P. K. Pujari *ChemPhysChem* 14 1055 (2013).
- [5] S. K. Sharma, J. Prakash, J. Bahadur, K. Sudarshan, P. Maheshwari, S. Mazumder and P. K. Pujari *Phys. Chem. Chem. Phys.* 16, 1399 (2014).
- [6] S. K. Sharma, J. Prakash, K. Sudarshan, D. Sen, S. Mazumder, P. K. Pujari. *Macromolecules* 48, 5706 (2015).
- [7] S. K. Sharma, J. Prakash and P. K. Pujari. *Phys. Chem. Chem. Phys.* 17, 29201 (2015).
- [8] S. K. Sharma, K. Sudarshan and P. K. Pujari. *Phys. Chem. Chem. Phys.* 18, 25434 (2016)
- [9] S. K. Sharma, J. Prakash, J. Bahadur, M. Sahu, S. Mazumder and P. K. Pujari. *European Polymer Journal* 84 100 (2016).
- [10] S. K. Sharma, K. Sudarshan, M. Sahu and P. K. Pujari *RSC Advances* 6, 67997 (2016).

PALS and ESR evidence of the dynamic crossover in the amorphous phase of the crystalline *n* - alkanes

J. Bartoš^{1,*}, B. Zgardzinska², H. Švajdlenková¹, M. Lukešová¹, R. Zaleski²

¹Polymer Institute of SAS, Dúbravská cesta 9, SK-845 41 Bratislava, Slovakia.

²Institute of Physics, M. Curie - Skłodowska University, PL-20031 Lublin, Poland

*e-mail: Jozef.Bartos@savba.sk

The *n*-alkanes form an important class of organics serving as models for polymers, surfactants and bio-systems. In spite of the simple chemical structure their thermodynamic and structural behaviors are rather very complex. The most significant complicated feature is their slight supercooling ability which leads to hardly achievable amorphous states of the *n*-alkanes. Consequently, basic descriptors of the amorphous *n*-alkanes or the amorphous states of the crystalline *n*-alkanes such as the glass-liquid transition at T_g and the dynamic crossover within the supercooled liquid at T_X require very special experimental and/or evaluation techniques. Thus, the former can be obtained by a vapor deposition technique for the shortest member only [1], while the latter follows as a parameter from the power law fit of the normal (fluid) liquid state viscosity also for the shorter members: *C3-C12* [2]. The aim of this contribution is to present a combined PALS and ESR study of both the annihilation behavior of the external atomic probe, *ortho*-positronium (*o*-Ps) and the related free volume and the reorientation dynamics of another external molecular probe, i.e., one of the smallest spin probe 2,2,6,6-tetramethyl-piperidiny-1-oxy (TEMPO) in typical even and odd *n*-alkanes: *n*-hexane (*C6*) and *n*-undecane (*C11*). In both the ESR and PALS responses, i.e. τ_3 vs. T and $2A_{zz}$ vs T plots, the main solid-liquid phase transition at T_m and for *C11* also the solid-solid phase transition at T_{ss} are confirmed in accord with the two *n*-alkanes studied by this combined approach so far: *n*-tridecane (*C13*) and *n*-hexadecane (*C16*) [3,4]. In addition, both PALS and ESR provide the corresponding evidences indicating the presence of amorphous domains within the crystalline phase of *C6* and *C11* and supporting the existence of the suggested crossover at T_X within the supercooled liquid state of the crystalline *n*-alkanes.

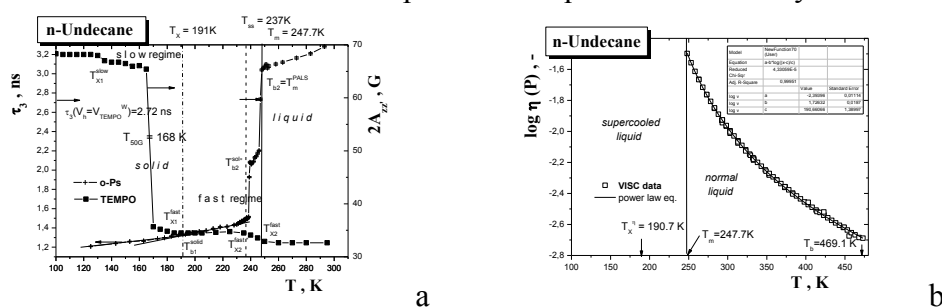


Fig.1. a. Comparison of ESR and PALS responses ; b. Power law fit of the liquid viscosity of *C11*.

- [1] K. Takeda, M. Oguni, J. Suga, *J Phys Chem Solids*, **8**, 991 (1991)
- [2] F. Mallamace, C. Branca, C.C. Corsaro, N. Leone, J. Spooren, S.H. Chen and H.E. Stanley, *PNAS* **107**, 22457 (2010)
- [3] M. Lukešová, B. Zgardzinska, H. Švajdlenková, R. Zaleski, B. Charmas, J. Bartoš, *Physica B Cond Matt* **476**, 100 (2015)
- [4] J. Bartoš, H. Švajdlenková, R. Zaleski, M. Edelmann, M. Lukešová, *Physica B Cond Matt* **430**, 99 (2013)

O17 | **Comparative study of positron- and electron stimulated ion desorption from a TiO₂ (110) surface**

T. Tachibana^{1*}, T. Yamashita¹, M. Nagira¹, H. Yabuki¹, L. Chiari^{1,2},
T. Hirayama³, and Y. Nagashima¹

¹*Department of Physics, Tokyo University of Science, 1-3 Kagurazaka, Shinjuku, Tokyo 162-8601, Japan*

²*Department of Applied Chemistry and Biotechnology, Faculty of Engineering, Chiba University, 1-33 Yayoi, Inage, Chiba 263-8522, Japan*

³*Department of Physics, Rikkyo University, 3-34-1 Nishi-Ikebukuro, Toshima, Tokyo 171-8501, Japan*

*e-mail: tachibana@rs.tus.ac.jp

When low energy positrons impinge on solid targets, they rapidly thermalize and diffuse in the bulk. Some of them reach the surface and annihilate predominantly with valence electrons. A small fraction of those positrons, however, may annihilate with core electrons, and in this case two or more electrons leave from the valence orbitals via an Auger decay process [1]. Thus, the fragmentation and desorption of ionic species from the surface may be caused by a Coulomb repulsion between the valence holes. While the bombardment of high energy positrons, as well as high energy electrons, can also lead to ion desorption via an impact excitation process, positron annihilation is the only possible desorption process for slow positrons with an incident energy below the desorption threshold by impact excitation.

Recently, we observed positron-stimulated ion desorption from a TiO₂(110) surface [2-4]. Desorbed O⁺ ions were clearly detected employing a modified time-of-flight (TOF) technique even in the incident positron energy range below the desorption threshold for electron impact [2], which corresponds to the ionization energy of Ti(3p) core electrons [5]. This result provided the evidence that core-hole creation by positron annihilation with inner-shell electrons leads to the O⁺ ion desorption.

In the present work, we have compared the positron- and electron-stimulated ion desorption. Considerable differences were found in the desorbed ion species and TOF distributions. Moreover, the desorption yield of the O⁺ ions for positron-stimulated desorption is one order of magnitude higher than that for electron-stimulated desorption. These results suggest that the positron surface states and the annihilation-site selectivity strongly affect the desorption process.

- [1] A. Weiss, R. Mayer, M. Jibaly, C. Lei, D. Mehl, and K.G. Lynn *Phys. Rev. Lett.* **61**, 2245 (1988)
- [2] T. Tachibana, T. Hirayama, and Y. Nagashima, *Phys. Rev. B* **89**, 201409(R) (2014)
- [3] T. Tachibana, T. Hirayama, and Y. Nagashima, *e-J. Surf. Sci. Nano tech.* **13**, 261 (2015)
- [4] T. Tachibana, L. Chiari, M. Nagira, T. Hirayama and Y. Nagashima *Def. Diff. For.* **373**, 324 (2016)
- [5] L. Knotek and P. J. Feibelman, *Phys. Rev. Lett.* **40**, 964 (1978)

O18 | **Structure determination of TiO₂ crystal surfaces using total-reflection high-energy positron diffraction (TRHEPD)**

I. Mochizuki¹, Y. Fukaya², H. Ariga³, R. Yukawa¹, K. Wada⁴, M. Minohara¹,
H. Kumigashira¹, K. Asakura³, A. Ichimiya¹, and T. Hyodo¹

¹ *Institute of Materials Structure Science, KEK, Tsukuba, 305-0801, Japan*

² *Advanced Science Research Center, JAEA, Tokai, 319-1195, Japan*

³ *Institute of Catalysis, Hokkaido University, Sapporo, 305-8569, Japan*

⁴ *Quantum Beam Science Center, QST, Takasaki, 370-1292, Japan*

* email: mochizu@psot.kek.jp

Single-crystal TiO₂ surfaces have been studied extensively as a testing ground for metal-, molecule-, and nanoparticle adsorptions [1, 2], providing opportunities to understand the catalytic reactions on an atomic level. Knowledge on their topmost- and subsurface structures, where catalytic processes occur, is critical factor in the understanding of the fundamentals and the reaction mechanisms of solid catalysts.

We investigated the structures of a rutile-TiO₂ (110) (1×2) [3] and of an anatase-TiO₂(001) (1×4) surfaces by means of a newly developed total-reflection high-energy positron diffraction (TRHEPD) apparatus [4, 5] at Slow Positron Facility, KEK, Japan. TRHEPD [6], the positron counterpart of reflection high-energy electron diffraction (RHEED), provides an exceedingly surface-sensitive tool for the structural determination [7]. The rutile-TiO₂ (110) (1×2) surface was as yet undetermined and widely discussed over the past 30 years. Our TRHEPD analysis [3] showed that the outermost atomic arrangement is explained by relaxing a basic structure of Ti₂O₃ composition [8] into an asymmetric configuration. This conclusion agreed well with a recent theoretical model [9] determined by a global optimization varying both composition and arrangement of the surface.

Successful formation of a single-crystal, vacancy-less anatase-TiO₂ (001)-(1×4) surface on a SrTiO₃ (001) crystal substrate was recently reported [10]. Several models have been proposed for this structure [2], based on surface-science techniques and/or theoretical calculations, but the rigorous atomic arrangement is yet to be settled. We report that the result of the TRHEPD experiment best matches that of the structural calculation assuming the “Ad-molecule model” [11] with some modifications of the atomic positions.

This study was conducted by the PF-PAC-approved proposals No. 2013U002, and 2016G072. This work was partly supported by Grant-in-Aid from JSPS for Scientific Research (S)24221007, Young Scientists (B)26800170, Young Scientists (B)17K14316, and Nippon Sheet Glass Foundation for Material Science Grant.

- [1] K. Asakura et al., Faraday Discuss. 162, 165 (2013)
- [2] U. Diebold, Surf. Sci. Rep. 48, 53 (2003)
- [3] I. Mochizuki et al., Phys. Chem. Chem. Phys. 18, 7085 (2016)
- [4] K. Wada et al., Eur. Phys. J. D 66, 37 (2012)
- [5] M. Maekawa et al., Eur. Phys. J. D 68, 165 (2014)
- [6] A. Ichimiya, Solid State Phenom. 29, 143 (1992)
- [7] Y. Fukaya et al., Appl. Phys. Express 7, 056601 (2014)
- [8] H. Onishi and Y. Iwasawa, Surf. Sci. 313, L783 (1994)
- [9] Q. Wang et al., Phys. Rev. Lett. 113, 266101 (2014)
- [10] T. C. Rödel et al., Phys. Rev. B 92, 041106 (2015)
- [11] M. Lazzeri and A. Selloni, Phys. Rev. Lett. 87, 266105 (2001)

O19 | Aerogel IC3120 under high pressure, obtained by pistons and nitrogen molecules

Marek Gorgol^{1,*}, Bożena Zgardzińska¹

¹ *Maria Curie-Skłodowska University, Institute of Physics, Department of Nuclear Methods,
Pl. M. Curie-Skłodowskiej 1, 20-031 Lublin, Poland*

*email: marek.gorgol@poczta.umcs.lublin.pl

Highly porous IC3120 silica aerogel was subjected to the high pressure up to 450 MPa, while the positron annihilation lifetime spectra were collected. The pressure was delivered to the investigated samples in two ways: by pistons and by gas (nitrogen) penetrating the aerogel. The evolution of all PALS parameters is discussed. With the increase of the pressure, shortening of orthopositronium lifetimes (different, depending on the pressure introducing method) is observed. Similarity between the dependence of the longest-lived o-Ps component's lifetime on the pressure, for the sample affected with nitrogen molecules and pure nitrogen was observed. It suggests, that the nitrogen fills the largest free volumes of aerogel. The pressure exerted on investigated aerogel mechanically, causes much smaller decrease of free volume available for positronium.

Comparison of PALS results with the electron microscopy images obtained after removing the pressure confirmed, that more intense and lasting changes were caused by affecting the aerogel with the pistons.

Positronium in mesopores of silica thin films

Chunqing He*

*Key Laboratory of Nuclear Solid Physics Hubei Province, School of Physics and Technology,
Wuhan University, Wuhan 430072, China*

* email: hecq@whu.edu.cn

Correctly evaluation of meopores by positron annihilation needs deep understanding of behaviours of positronium (Ps) atoms in mesopores. In this talk, positronium behaviors in pores of various mesoporous silica thin films, deposited on Si wafers via a sol-gel method using either triblock copolymers or a cationic surfactant as structure-directing agents, were studied by positron annihilation spectroscopes based on slow positron beams. Pore surface chemistry, interconnectivity and morphology on Ps diffusion, annihilation characteristics in mesopores are reviewed[1-7]. Ps lifetime in mesopores is associated with pore size, pore geometry and pore surface chemistry. Ps emission/3g annihilation depends not only on the pore interconnectivity but also on pore morphologies due to Ps localization in larger pores. Because of the nature of Ps confinement in nano-channels, orientation of tubal pores could be distinguished by measuring S, W parameters of positron annihilation in ordered pores aligning along silica film surface using Doppler Broadening of annihilation radiation (DBAR). This makes it possible to evaluate morphologies of mesopores both in silica films and around the interface between the silica film and Si substrate.

This work was supported in part by National Natural Science Foundation of China (NSFC) under Grants 11375132&11575130.

- [1] C. He, et al., *Phys. Rev. B.* **75**, 195404 (2007).
- [2] C. He, et al., *Appl. Phys. Lett.* **91**, 024102(2007).
- [3] C. He, et al., *Phys. Rev. B.* **86**, 075415 (2012).
- [4] C. He, et al., *Chem. Phys. Lett.* **590**, 97 (2013).
- [5] B. Xiong, et al., *J. Appl. Phys.* **115**/9, 094303 (2014).
- [6] B. Xiong, et al., *Phys. Lett. A.* **378**, 249 (2014).
- [7] X. Tang, et al. *Electrochimica Acta* **168**, 365 (2015).

Nanopore structure of siloxane-silica CVD films elucidated by the low-energy AMOC technique with a radioisotope-based pulsed positron beamK. Ito*National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki
305-8565, Japan*

*email: k-ito@aist.go.jp

The positronium (Ps) lifetime technique is well documented as a sensitive tool for probing nanometer-scaled open-space in various oxides and polymers [1,2], in order to elucidate their macroscopic properties such as molecular permeability [3] and ion transport [4]. Our group has so far reported on the usefulness of this technique for investigating free-volume holes/nanopores in a variety of functional materials like separation membranes [4,5], hydrophilic polyolefins [6], and silica films [7]. In 2003, our group proved that the positron and Ps momentum distributions for polymers associate with their constituent elements [8], suggesting that Ps may be useful for probing the chemistry of free-volume surfaces. For instance, 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 the chemical analysis around the free volumes [9].

In this work, an energy-tunable AMOC measurement system with a radioisotope-based pulsed positron beam was developed for investigating functional thin materials. Positron annihilation lifetime spectroscopy (PALS) was performed using a positron pulsing system (FUJI IMVAC Inc., Japan) with a time resolution of about 250 ps (FWHM), and Doppler broadening of positron annihilation radiation (DBAR) was measured using a high-purity Ge detector with an energy resolution of 1.63 keV at 1.33 MeV and an efficiency of 39 %. In order to obtain AMOC data, coincidence signals from PALS and DBAR were stored in a PC using a digital signal-processing module developed by TechnoAP, Japan. As the first application, siloxane-silica hybrid thin films, fabricated through plasma-enhanced chemical vapor deposition [7], were examined using the developed system. The effect of the siloxane monomer content on the free-volume structure was discussed based on the AMOC data. Details of the measurement system and obtained results are presented at the workshop.

This work was supported by JSPS KAKENHI Grant Number 16H04526.

- [1] K. Ito, H. Nakanishi, Y. Ujihira, *J. Phys. Chem. B*, 103 (1999) 4555.
- [2] K. Ito and Y. Kobayashi, *Acta Phys. Pol. A*, 107 (2005) 717.
- [3] K. Ito, Y. Saito, T. Yamamoto, Y. Ujihira, K. Nomura, *Macromolecules*, 34 (2001) 6153.
- [4] Z. Chen, K. Ito, H. Yanagishita, N. Oshima, R. Suzuki, Y. Kobayashi, *J. Phys. Chem. C*, 115 (2011) 18055.
- [5] T. Niimi, H. Nagasawa, M. Kanezashi, T. Yoshioka, K. Ito, T. Tsuru, *J. Membr. Sci.*, 455 (2014) 375.
- [6] H. Hagihara, K. Ito, S. Kimata, *Macromolecules*, 46 (2013) 4432.
- [7] K. Ito, T. Oka, C. He, Y. Kobayashi, *JJAP Conference Proceedings*, 2 (2014) 011210.
- [8] K. Ito, Y. Kobayashi, A. Nanasawa, *Appl. Phys. Lett.*, 82 (2003) 654.
- [9] K. Sato, H. Murakami, K. Ito, K. Hirata Y. Kobayashi, *Macromolecules*, 42 (2009) 4853.

Free-volume evolution in 1-propanol confined in partially filled regular mesopores of SBA- 15 matrixO. Šauša^{1,*}, M. Lukešová², H. Švajdlenková² and J. Bartoš²¹*Institute of Physics, Slovak Academy of Sciences, Dúbravská cesta 9, 845 11 Bratislava, Slovakia*²*Polymer Institute, Slovak Academy of Sciences, Dúbravská cesta 9, 845 41 Bratislava, Slovakia**email: ondrej.sausa@savba.sk

1-propanol belongs to polar substances with a simple structure and significant use in synthetic, solution organic and polymer chemistry. It serves as an important prototypical polar protic organic compound in various types of condensed matter studies.

The aim of this work was to show the changes in the annihilation behavior of ortho-positronium (oPs) in 1-propanol confined in regular mesopores of the SBA-15 matrix as compared to the bulk state [1] with temperature as well as differences in its free-volume evolution at the different levels of pore filling. Since the SBA-15 matrix is a hard inorganic matrix with a polar inner surface, we anticipate the manifestations of the attractive interactions between the polar groups of 1-propanol and the SBA-15 matrix in filling the matrix mesopores as well as in the free-volume microstructure of the confined 1-propanol.

From the measured dependencies of the oPs lifetimes and their relative intensities on the filling coefficient k ($k = M_{\text{prop}}/M_{\text{tot}}$, where M_{prop} is the weight of propanol and M_{tot} is the weight of the matrix together with the confined propanol) is shown that the gradual filling of the mesopores with molecules of 1-propanol is most likely first by bonding the 1-propanol molecules to the inner polar surface in the thin layer and then filling the pores completely. In addition, at some significant filling coefficients, the free-volume properties of 1-propanol were measured over a wide temperature range of 15-350 K. Filling coefficients $k=0.15$, 0.24 and 0.35 were chosen at which the changes in oPs lifetimes or their relative intensities occur, measured at room temperature.

[1] J. Bartoš, H. Švajdlenková, O. Šauša, M. Lukešová, D. Ehlers, M. Michl, P. Lunkenheimer and A. Loidl, *J. Phys.-Cond. Matt.* **28**, 015101 (2016)

O23 | **Slow positron annihilation spectroscopy of mesoporous silicon oxide films obtained by electro-assisted self-assembly**

 B. Y. Wang^{1,*}, C. Q. He², X. W. Zhang², P. Kuang¹, and X. Z. Cao¹
¹ *Institute of High Energy Physics, Chinese Academy of Sciences, 100049 Beijing, China*
² *School of Physics and Technology, Wuhan University, Wuhan, 430072 Hubei, China*

*email: wangboy@ihep.ac.cn

Supported mesostructured thin films are of major importance for applications in optical, electrochemical and sensing devices. Highly ordered and vertically oriented mesoporous silica oxide films can be generated by electro-assisted self-assembly (EASA). The method involves the electrogeneration of hydroxide ions at an electrode surface immersed in an hydrolyzed sol solution (containing typically tetraethoxysilane, TEOS, and cetyltrimethylammonium bromide, CTAB) in order to catalyze polycondensation of the precursors and self-assembly of hexagonally packed one-dimensional channels that grow perpendicularly to the support (ITO). Thickness of these films can be accurately controlled by applying galvanostatic conditions and by varying the deposition time. However, the influence of the CTAB/TEOS concentration ratio on the mesoporous structure has never been thoroughly examined. Slow positron annihilation spectroscopy is a powerful tool to study in-depth variation of membrane fine structural. In this paper, we report a combined study of the Doppler broadening (DBES) and positron annihilation lifetime spectroscopy (PALS) methods coupled with variable monoenergy slow positron beams to study the positron annihilation characterization in mesoporous silicon oxide films (200nm) formed with four different CTAB/TEOS ratios. The S-W curve shows that there are three straight line segments, respectively, corresponding to the three transition regions of the film. Obviously, the S parameter of the transition zone from the silicon oxide film to the interface between the silicon oxide and the ITO significantly changes with different CTAB/TEOS ratios, indicating the mesoporous structure of films can be well regulated by modifying its ratio. The long lifetime of positron lifetime spectra correlating to magnitude of nanosecond order indicates that the film of CTAB/TEOS ratio 0.04 has the largest mesoporous size.

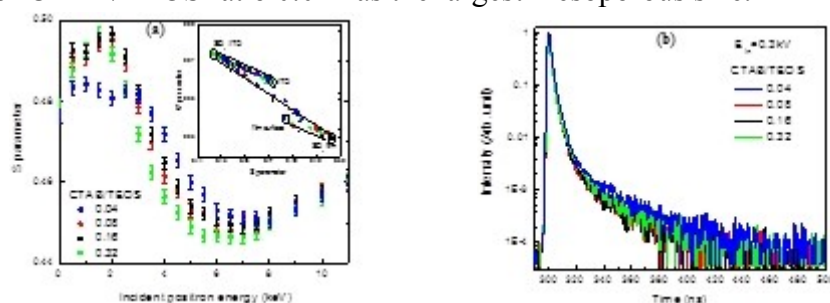


Fig (a). S parameter and S-W plot of 200nm-thin films. Arrows show the incident positron energy E_{in} from 0.012 keV to 10 keV; Fig (b). The PALS with when incident positron energy was 0.3 keV.

Acknowledgements

This work is supported by National Natural Science Foundation of China (11575205).

[1] Yamaguchi, A. et al. *Nature Mater.* **3**, 337–341 (2004)

[2] Deepa, P. N., Kanungo, M., Claycomb, G., Sherwood, P. M. A. & Collinson, M. M. *Anal. Chem.* **75**, 5399–5405 (2003)

O24 | **Investigation of the porous structure of oblique angle deposited thin films with tailored architectures**

M. Butterling^{1,*}, A.R. González-Elipé², M.O. Liedke¹, A.G. Valenzuela², R. Alvarez², A. Palmero², J. Gil-Rostra², V. Rico-Gavira², E. Hirschmann^{1,3}, R. Krause-Rehberg³, M. Kraatz⁴, and A. Wagner¹

¹*Institut für Strahlenphysik, Helmholtz-Zentrum Dresden - Rossendorf, Dresden, Germany*

²*Laboratory of Nanotechnology on Surfaces, Instituto de Ciencia de Materiales de Sevilla (CSIC-Universidad de Sevilla), Seville, Spain*

³*Insitut. für Physik, Universität. Halle, Halle, Germany*

⁴*Fraunhofer Institute for Ceramic Technologies and Systems (IKTS), Dresden, Germany*

*email: m.butterling@hzdr.de

Oblique angle deposited (OAD) thin films offer many possibilities for tailoring their microstructure for specific applications, which are typically linked with the high fraction of void space and porosity available in these thin films (typically of 50% or more from the total volume of the films) and the possibility of tailoring their microstructure in the form of slanted, chiral, zig-zag or similar nanostructures [1]. Combining these films in the form of multilayers of different materials open additional ways for tailoring their microstructure and the development of new properties for advanced applications [2], e.g., optofluidic sensors, fuel cells and many others. For all these applications, control of the porous structures is essential and a precise knowledge is required of the porous structure, the interconnection between open pores, the possibility of creating close pores, etc.

Here, we will present the first results for the investigation of three different nano-columnar systems: single element (i) SiO₂ (Fig. 1) and (ii) TiO₂ films, and (iii) SiO₂/TiO₂ multilayers, which have been studied by means of Doppler broadening (DB) and positron annihilation lifetime spectroscopy (PALS) using the MePS facility at HZDR. *Three* different pore populations have been detected for SiO₂ nano-columns, *two* for multilayers and only *one* pore size for TiO₂. Pore size distribution evaluated by the MELT code will be given.

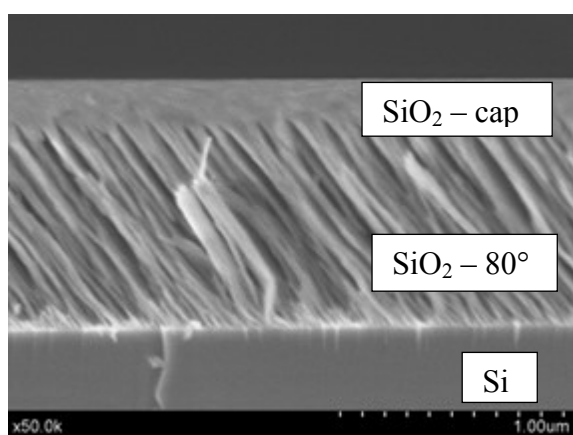


Fig. 1 Cross-sectional SEM image of e-beam evaporated SiO₂ nano-columnar film (about 1 μm thick), capped with about 200 nm thick compact SiO₂ layer.

[1] A. Barranco *et al.*, *Mater. Sci.* **76** 59 (2016)

[2] M. Oliva-Ramirez *et al.*, *ACS Nano* **10**, 1256 (2016) DOI: 10.1021/acsnano.5b06625

In-situ investigations of the curing process in ultra low-k materials

M.O. Liedke^{1,*}, N. Koehler², M. Butterling¹, A.G. Attallah³, R. Krause-Rehberg³, E. Hirschmann^{1,3}, S.E. Schulz^{2,4} and A. Wagner¹

¹*Institut für Strahlenphysik, Helmholtz-Zentrum Dresden - Rossendorf, Dresden, Germany*

²*Zentrum für Mikrotechnologien, Tech. Univ. Chemnitz, Chemnitz, Germany*

³*Institut für Physik, Universität Halle, Halle, Germany*

⁴*Fraunhofer ENAS, Technologie-Campus 3, Chemnitz, Germany*

*email: m.liedke@hzdr.de

Porous spin-on glasses belong to ultra low-k (ULK) dielectrics and are promising candidates for integration in the semiconductor device fabrication technology. Their microstructure consists usually of interconnected pore networks distributed across the film rather than separated voids. The pore size and distribution are controllable to a large extent, however, the pore formation process itself is still not well understood. A dielectric damage during integration and material degradation of films with large porosity are still problematic issues. The first results on in-situ investigations of the pore formation during a curing process – a porogen removal by vacuum annealing will be presented. The main motivation is to obtain the insight into early stages of the pore formation and up to its full development. The in-situ annealing and Doppler Broadening – Positron Annihilation Spectroscopy (DB-PAS) measurements have been done on our Apparatus for In-situ Defect Analysis (AIDA) system [1], which is the end-station of the slow positrons beamline at HZDR. The comparison between preliminary ex-situ studies by means of DB-PAS [see Fig. 1], Positron Annihilation Lifetime Spectroscopy (PALS), and Fourier Transform Infrared Spectroscopy (FTIS) will be given.

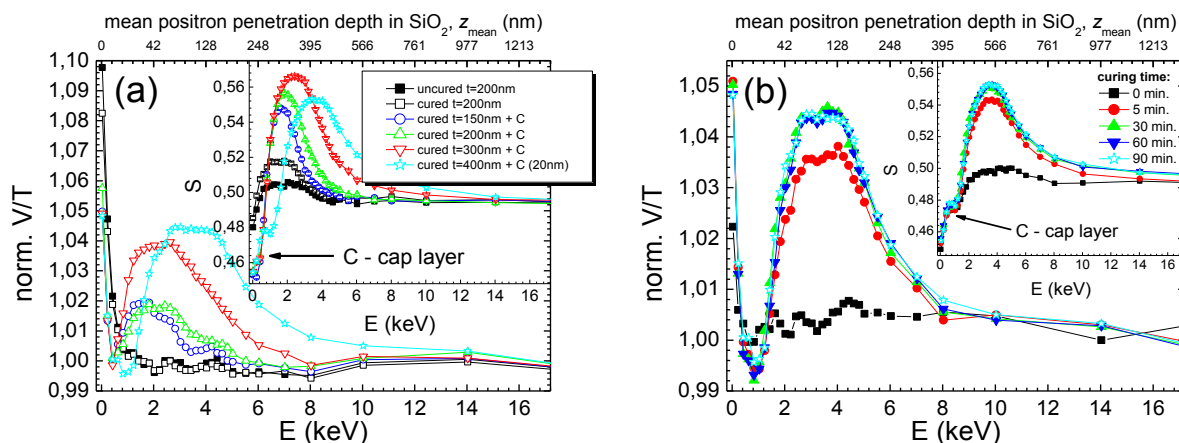


Fig. 1. ortho-Positronium (o-Ps) emission [norm. to bulk V/T parameter] as a function of positron implantation energy, E and mean positron penetration depth, z_{mean} for samples with different (a) thicknesses, t and (b) curing times for t=400nm [450°C, 1h]. Cured samples with the ULK film thickness variation were capped with a carbon layer (10nm thick for t<400nm, and 20nm for t=400nm). In (b) all the samples were capped with 20nm C. S-parameter as a function of E (insets).

In Fig. 1(a) it is shown that o-Ps emission increases with t, thus can be a probe of films porosity as long as they are capped. The curing time of 5-30min. is sufficient to fully develop the pore network [Fig. 1(b)]. Porosity development and distribution will be discussed for annealing temperatures in the 100-400°C range and varied annealing time.

[1] M.O. Liedke et al., *Journal of Applied Physics* **117**, 163908 (2015).

O26 | **Porosimetry of ultra-low K materials and transformed porous glass-thin layers by Monenergetic Positron Source at ELBE facility**

A. G. Attallah^{1,2*}, N. Koehler³, G. Dornberg⁴, M. Butterling⁵, M.O. Liedke⁵, A. Wagner⁵, S.E. Schulz^{3,6}, E. Badawi², D. Enke⁴ and R. Krause-Rehberg¹

¹ *Institut für Physik, Martin-Luther-Universität Halle, 06099 Halle, Germany*

² *Physics Department, Faculty of Science, Minia University, 61519 Minia, Egypt*

³ *Zentrum für Mikrotechnologien, TU Chemnitz, 09126 Chemnitz, Germany*

⁴ *Institut für Technische Chemie, Universität Leipzig, 04103 Leipzig, Germany*

⁵ *Institut für Strahlenphysik, HZDR, 01314 Dresden, Germany*

⁶ *Fraunhofer ENAS, Technologie-Campus 3, 09126 Chemnitz, Germany*

* email: agamal86_physics@yahoo.com

The pore size of spin-on coated ultra-low K (ULK) materials cured at 450⁰C for different times was studied by the pulsed slow positron beam (MePS) at ELBE/HZDR. To investigate the pore formation in cured porous spin-on dielectrics, the pore size as a function of positron implantation energy was obtained for samples with different curing times. Such a study is performed to understand the dielectric damage behaviour of ULK dielectrics for the integration in Back-End of Line (BEOL). MePS results revealed that the films contain open and closed pores with ~ 3 nm in diameter which was confirmed by capping the samples. The highest pore concentration is located beneath the surface in the 0.2 - 0.5 μm range (We plan to carry out ellipsometric porosimetry and FTIR during this summer). Pseudomorphic transformation of porous glass-thin layers, with pores of 40 - 50 nm diameter and a relatively small surface area, to MCM-41 with ~4 nm pores, with a higher surface area, was studied by MePS. The small pore size of MCM-41 was successfully detected with an intensity growth with transformation degree but the large pores were not detected at all. To understand the disability of detecting the large pores by positron annihilation lifetime, we plan to perform SEM measurements in the same depth as that of the implanted positrons (0.005-2.4 μm). Additionally, the increase in the intensity of positronium lifetime, which correlates the small pores, as a function of positron implantation energy could reflect inner pore isolation or poor interconnectivity.

O27 | Pores in highly densified silica glass by positron annihilation spectroscopy

M. Fujinami^{1,*}, S. Aoyama¹, M. Ono² and S. Ito²¹Department of Applied Chemistry, Chiba University, 1-33 Yayoi, Inage, Chiba, Japan²Asahi Glass Co. Ltd., Hazawa, Kanagawa, Yokohama 221-8755, Japan

*email: fujinami@faculty.chiba-u.jp

Pores are greatly related to the properties of silica glasses. We have previously examined voids in silica glasses with different fictive temperatures using positron annihilation lifetime spectroscopy (PALS) [1]. The pick-off annihilation lifetime of o-Ps increased with the fictive temperature, T_f , although the density increased. Further, it was found that this result was very similar to that of the Rayleigh scattering coefficient. High T_f leads to a low degree of network polymerization, resulting in a large density fluctuation. Therefore, the largest pores appeared in the silica glass at high T_f and o-Ps was able to detect such large pores. In this work, highly densified silica glass specimens were produced using the hot isostatic pressure (HIP) method. PALS and Rayleigh scattering measurements were then carried out on those samples.

Highly densified silica glass specimens with ϕ 50 mm and 70 mm length were manufactured using the HIP method. The temperature was 2073 K and the atmosphere was Ar gas. The pressure was varied from 0.1 MPa to 200 MPa with a preparation time of up to 4 h. For the sample prepared at 200 MPa, the refractive index and the density saturated within 1 h, while the o-Ps lifetime and Rayleigh scattering coefficient gradually decreased within the preparation time of up to 4 h. This meant that the macroscopic properties did not change for more than 1 h, but the relaxation of the microscopic pore structures continued for a longer time. The plot of Rayleigh scattering intensity versus pore radius estimated from the o-Ps lifetime is summarized in the figure below. This figure shows a good correlation between the two. It was found that the highly densified silica glass showed a small density fluctuation and the pores detected by o-Ps became smaller. We, thus, conclude that PALS is a suitable method for estimating the pore size in silica glasses.

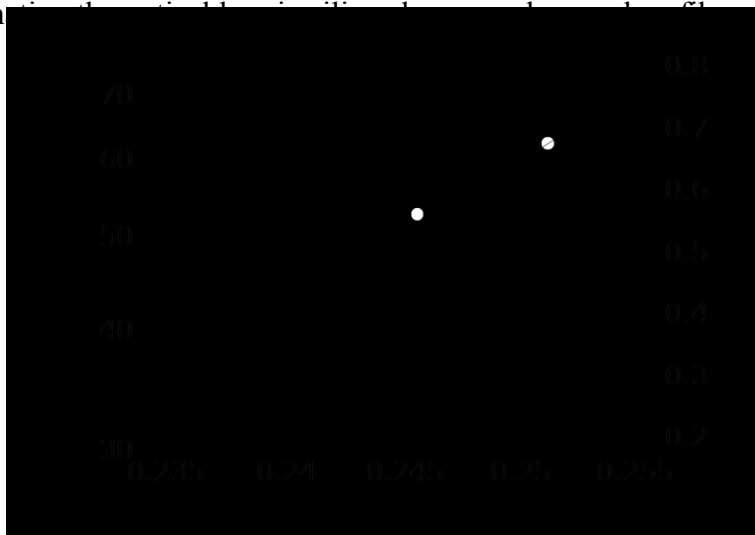


Fig. Rayleigh scattering intensity versus pore radius estimated from the o-Ps lifetime.

[1] M. Ono, K. Hara, M. Fujinami, and S. Ito, *Appl. Phys. Lett.* **101**, 164103 (2012)

Effect of heat treatment on the nanoporosity of silica PECVD films elucidated by the low-energy positron lifetime technique and ellipsometric porosimetry

S. Yoshimoto^{1,3,*}, K. Ito², H. Hosomi¹, M. Takeda¹, T. Tsuru³

¹ Toray Research Center, Inc., 3-3-7 Sonoyama, Otsu, Shiga 520-8567, Japan

² National Institute of Advanced Industrial Science and Technology (AIST), 1-1-1 Higashi, Tsukuba, Ibaraki 305-8565, Japan

³ Hiroshima University, 1-3-2 Kagamiyama, Higashi-Hiroshima, Hiroshima 729-8527, Japan

* email: Shigeru_Yoshimoto@trc.toray.co.jp

Engineering the nanoporosity of silica thin films is important to improve the functionality of various materials for sensors, separation membranes, etc. One method to control the porosity is heat treatment of the films, which can modify the silica networks, so that the pore structure is altered at the molecular level. In this study, low-energy positron annihilation lifetime spectroscopy (PALS) and ellipsometric porosimetry (EP)[1][2] were applied to the evaluation of the nanopores in silica thin films fabricated by plasma-enhanced chemical vapor deposition (PECVD). The effect of the heat treatment on the nanoporosity was investigated.

Silica films with a thickness of 400 nm were deposited at 300°C on silicon wafers with different flow rate ratios of the oxygen and tetraethyl orthosilicate (TEOS) precursors. Refractive indices for the as-deposited silica films, a measure of the film density, decreased with increasing TEOS fraction, suggesting suppressed development of the silica networks due to the excess amount of TEOS in the precursor. PALS results showed that their pore sizes, quantified from the ortho-positronium lifetimes, increased from 0.30 nm to 0.35 nm in radius with decreasing refractive index, indicating that the pore sizes were associated with the film total porosity. The films were annealed at 550°C under a dried nitrogen flow. While the total porosity, estimated from the refractive index, was not significantly changed with the heat treatment (Fig. 1), open porosity for the annealed films was not observed by EP with methanol (Fig. 2). This means that the connected pores accessible to the methanol molecule were isolated by annealing at 550°C. Details including the positron results for the annealed films will be discussed in the presentation.

This work was supported by JSPS KAKENHI Grant Numbers 15H02313, 16H04526.

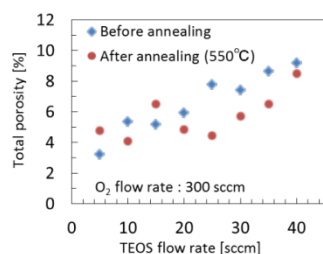


Fig. 1 Relationship between the total porosity and the TEOS fraction for the dry silica films.

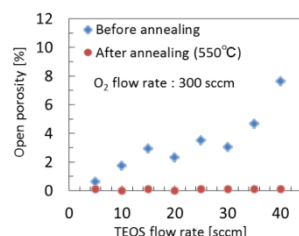


Fig. 2 Relationship between the open porosity and the TEOS fraction for the silica films.

[1] S. Yoshimoto, K. Ito, H. Hosomi and Y. Takai, J. Appl. Phys. Conf. Proc. 2 (2014) 011205

[2] S. Yoshimoto, K. Ito, H. Hosomi, T. Nakamura and M. Takeda, J. Phys: Conf. Proc., 791 (2017) 012027

Positronium formation in nanostructured metals

J. Čížek^{1,*}, O. Melikhova¹, P. Hruška¹, M. Vlček¹, W. Anwand², O. Liedke²,
M. Novotný³, J. Bulíř³ and Y. Cheng⁴

¹*Faculty of Mathematics and Physics, Charles University,
V Holešovičkách 2, 18000, Praha 8, Czech Republic*

²*Institute of Radiation Physics, Helmholtz-Zentrum Dresden-Rossendorf
Bautzner Landstr. 400, 01328 Dresden, Germany*

³*Institute of Physics, Academy of Sciences of the Czech Republic,
Na Slovance 2, 182 21 Prague 8, Czech Republic*

⁴*State Key Lab. of Solidification Processing, Northwestern Polytechnical University,
710072, Xi'an, P.R. China*

*email: jakub.cizek@mff.cuni.cz

Nanostructured metals containing nano- and micro-cavities can be prepared by various methods. Morphology of cavities can be controlled by varying the parameters of preparation. This enables fabrication of nanostructured metals with properties tailored for particular applications, e.g. nanostructured metals containing fractal-like cavities with a wide size distribution are used as omnidirectional absorbers of light from the visible into the infrared spectral region. Positronium (Ps) is a non-destructive probe of nanoscopic cavities capable of precise determination of their size distribution. In conventional metals Ps does not form since any bound state of positron and electron is quickly destroyed by the screening of conduction electrons. However, a thermalized positron escaping from a metal through inner surface into a cavity may form Ps by picking an electron on the surface. This process was examined in the present work on nanostructured metals prepared three various methods: (i) thin films of black metals (Au and Al) evaporated in N₂ atmosphere; (ii) nano-porous bulk Pd prepared by electrochemical etching of PdCo alloy; (iii) nanostructured Gd prepared by selective evaporation of Mg from MgGd alloy. Our investigations confirmed that Ps was formed in nanostructured metals. The the size distribution of nano-pores in the samples has been determined. The mechanism of Ps formation in these samples is discussed in the paper.

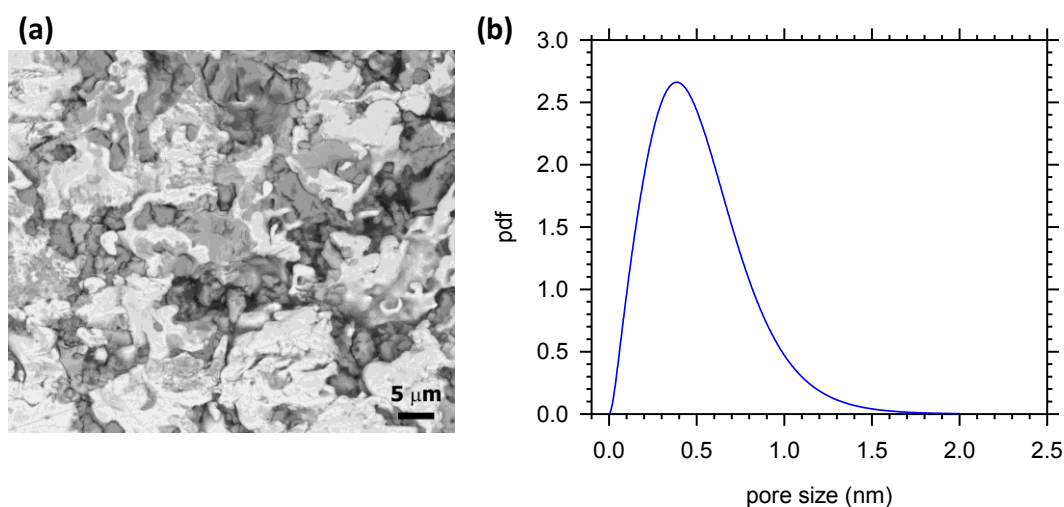


Fig.1. (a) SEM micrograph of nanostructured Gd prepared by selective evaporation of MgGd alloy; (b) size distribution of nanoscopic pores determined from pick-off annihilation lifetime of ortho-Ps.

O30 | Nucleation and growth of helium-vacancy clusters in ferritic-martensitic steels – effect of dpa rate

V. Krsjak^{1*}, S. Sojak¹, J. Degmova¹, V. Slugen¹

¹ *Institute of Nuclear and Physical Engineering, Faculty of Electrical Engineering and Information Technology, Slovak University of Technology in Bratislava, Ilkovicova 3, 81219 Bratislava, Slovakia*

*email: vladimir.krsjak@stuba.sk

Fe-12Cr model alloy implanted by helium ions was investigated in a context of Fe-9Cr steel irradiated in a mixed neutron-proton spectrum of spallation target. Application of pulsed low-energy positron beam enabled a careful selection of a region in the Bragg peak with the He concentration and displacement damage comparable to spallation conditions. The investigated samples, irradiated in Swiss Spallation Neutron Source – SINQ received up to 20dpa and 2000appm He in 2 years. A similar dose was obtained in the implanted samples in 72 hours. Despite a major acceleration of the displacement damage production, the positron lifetime data were found to be relatively comparable. However, the implanted samples show a more significant trapping at vacancy clusters with lifetime 200-280ps. Also, the absolute value of the positron lifetimes in this range of clusters was found to be larger in He-implanted samples. This suggests a higher concentration of vacancy clusters containing less helium in these samples, comparing to the spallation ones. More defects surviving cascade collisions can be explained by a presence of interstitial helium in the matrix, it's fast migration into radiation-induced vacancies and stabilization of these defects against recombination.

O31 | **High entropy HfNbTaTiZr alloys: structure stability, short range order and vacancies**

J. Kuriplach^{1,*}, J. Čížek¹, O. Melikhova¹, F. Lukáč², J. Zýka³ and J. Málek³

¹*Department of Low Temperature Physics, Faculty of Mathematics and Physics, Charles University, V Holešovičkách, CZ-18000 Prague 8, Czech Republic*

²*Department of Materials Engineering, Institute of Plasma Physics of the Czech Academy of Sciences, Za Slovankou 1782/3, CZ-18200 Prague 8, Czech Republic*

³*UJP PRAHA a.s., Nad Kamínkou 1345, CZ-15610 Prague - Zbraslav, Czech Republic*

*email: jan.kuriplach@mff.cuni.cz

High entropy (HE) alloys (HEAs) consist of several – usually at least four or five – components with nearly equiatomic concentrations [1]. “High entropy” in their name comes from the fact that they show a very large configurational entropy, which contributes to their stability. Such alloys started to attract attention – both from the scientific and applicational viewpoints – just a few years ago because of their unique properties, mainly mechanical and electrochemical ones. The properties of HE alloys are nowadays intensively studied, but investigations of defects are seldom. Positron annihilation (PA) may thus reveal details about open volume defects, and thereby about HEA microstructure related to HEA properties. HE alloys are not dilute but rather concentrated alloys. This fact has also consequences for positron annihilation research: Even simple defects like vacancies exist in many different atomic configurations. In addition, the “bulk” lifetime is not represented by a discrete value but exhibits a distribution with a certain (nonzero) width.

The HfNbTaTiZr high entropy alloy was discovered/introduced in 2011 [2] in quest of suitable materials for high temperature applications in the aerospace industry. All constituting elements are refractory metals, and so is the resulting alloy. The HfNbTaTiZr alloy displays excellent mechanical properties, like yield strength, but its defect structure is unknown to a large extent. In the present study, we first examine the phase stability of the HfNbTaTiZr alloys which crystallize in the bcc structure. We also attempt to determine the short-range order in these alloys using *ab initio* modelling based on a Monte Carlo approach [3]. The basic properties of single vacancies in the bulk are also investigated, including the possibility of the existence of structural vacancies. Finally, the first experimental PA results for HfNbTaTiZr samples produced by arc melting are shown and discussed with the help of computed positron characteristics for the bulk and vacancies.

[1] High-Entropy Alloys: Fundamentals and Applications, edited by M.C. Gao, J.-W. Yeh, P.K. Liaw and Y. Zhang, Springer (2016)

[2] O.N. Senkov et al., J. Alloys Comp. **509**, 6043 (2011)

[3] N. Metropolis et al., J. Chem. Phys. **21**, 1087 (1953)

Defect range and evolution in swift Xe-ion irradiated pure silver and titanium studied by positron annihilation techniquesJ. Dryzek^{1,*}, P. Horodek^{1,2}¹*Institute of Nuclear Physics Polish Academy of Sciences, PL-31342 Krakow, Poland.*²*Joint Institute for Nuclear Research, Joliot-Curie 6, 141980 Dubna, Moscow region, Russia*

*email: jerzy.dryzek@ifj.edu.pl

Positron annihilation spectroscopy is widely used for open volume defects identification in metals, alloys, semiconductors and other. However, it can be also applied for determination of defect spatial distribution in samples exposed to the surface treatment. This allows us to observe and recognize processes accompanying different treatments. The lecture will address the heavy ions implantation studied by positron annihilation spectroscopy including investigations performed by the author.

Implantation of energetic ions have been widely used to modify properties of the near surface region. It is important to understand the defect production, annihilation and migration mechanisms during and after collision cascades. In our studies, polycrystalline pure titanium and silver were irradiated by Xe²⁶⁺ ions with kinetic energy of 167 MeV and different doses. Slow positron beam and positron lifetime were used for detection of defects. We intend to focus on the total range of defects after irradiation. For this purpose we applied with success the sequenced etching technique which was previous used for detection of subsurface zone created during sliding (see e.g., [1]). Despite the small range of the Xe²⁶⁺ implantation, i.e., 10 μ m this technique allows to detect the defect depth profile induced by irradiation. The profile range coincidences with the range of ion calculated using SRIM/TRIM code. However, the shape of defect profile does not coincidence with this calculated from the code. No Bragg peak at the end of the range is observed. We will discuss also the so called long range effect. This effect predicts the expansion of defects beyond the ion implantation range [2, 3]. The slow positron beam results for these samples will be also presented.

[1] J. Dryzek, M. Wróbel, Tribol. Lett. **55**, 413 (2014)[2] Yu. P. Sharkeev, B.P.Gritsenko, A.V. Fortuna, A.J. Perry, Vacuum, **52**, 247 (1999)[3] Yu. P. Sharkeev, E.V. Kozlova, Surf. Coat.Technol. **158–159**, 219–224 (2002).

O33 | PAS studies applied for evaluation of neutron and hydrogen treated reactor steels

V. Slugen^{*}, S. Pecko, T. Brodziansky, S. Sojak, V. Krsjak, M. Petriska, J. Simeg Veternikova, and M. Saro

Institute of Nuclear and Physical Engineering, Slovak University of Technology, Ilkovičova 3, 81219 Bratislava, Slovakia

^{*}email: Vladimir.slugenr@stuba.sk

The safe operation of nuclear facilities is limited by neutron embrittlement of most loaded parts. Nuclear materials degradation caused by radiation exposure can be experimentally measured with difficulties connected to high radiation and manipulation. Based on long term experiences we focused also on experimental simulation of irradiation via ion implantation. In our case, German reactor pressure vessel (RPV) steels were studied by positron annihilation lifetime spectroscopy (PALS). This unique non-destructive method can be effectively applied for the evaluation of microstructural changes and for the analysis of degradation of reactor steels due to neutron irradiation and proton implantation. Studied specimens of German reactor pressure vessel steels are originally from CARINA/CARISMA program as well as Slovak surveillance specimen program (1995-2015). Actually eight specimens were measured in as-received state and two specimens were irradiated by neutrons in German experimental reactor VAK (Versuchsatomkraftwerk Kahl) in the 1980s. One of the specimens which was in as-received and neutron irradiated condition was also used for simulation of neutron damage by 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 “as-received” steels. A significant increase in the size of the induced defects due to neutron damage was observed in the irradiated specimens resulting in 2-3 vacancies. The size and intensity of defects reached a similar level as in the specimens irradiated in the nuclear reactor due to the implantation of hydrogen ions with energies of 100 keV (up to the depth <500 nm). Actual results from German reactor steels were compared to previous experiences with Russian and Japan reactor steels studied after different loads.

[1] H. Hein, E. Keim, H. Schnabel, T. Seibert, A. Gundermann, J. ASTM Int. 6 (2009) Paper ID JAI101962

[2] V. Slugeň, Safety of VVER-440 Reactors – Barriers Against Fission Products Release, Springer, 2011, ISBN 978-1-84996-419-7

[3] V. Slugen, V. Krsjak, W. Egger, M. Petriska, S. Sojak and J. Vetrenikova, J. Nucl. Mater. 409 (2011) 163

Investigation of near-surface radiation defects in Si and W by means of conventional positron lifetime spectrometer with a ²²Na positron source

Dubov L.Yu.^{1,2}, Akmalova Yu.A.¹, Stepanov S.V.^{1,2},
Ogorodnikova O.V.¹, Yu.V. Funtikov², Shtotsky Yu.V.^{1,2}

¹ National Research Nuclear University "MEPhI", Moscow, Russia

² NRC "Kurchatov Institute" - Institute for Theoretical and Experimental Physics, Russia

*email: lydubov@mephi.ru

In this work we studied near-surface defects in silicon irradiated by protons and in tungsten irradiated by W⁶⁺ ions by means of positron annihilation lifetime spectroscopy (PALS) using a ²²Na positron source. These studies require knowledge of positron implantation profiles in matter. We simulated them using GEANT4 toolkit. Positron implantation profiles can be approximated by the sum of two exponential functions:

$$f(x) = 0.11 \cdot a \cdot e^{-ax} + 0.89 \cdot b \cdot e^{-bx}, \quad (1)$$

where $a=0.11$, $b=0.012 \mu\text{m}^{-1}$ for silicon and $a=1.52$, $b=0.11 \mu\text{m}^{-1}$ for tungsten.

Fig. 1 shows implantation profiles of positrons from ²²Na source along with depth distributions of primary radiation defects (Frenkel pairs) calculated using SRIM program.

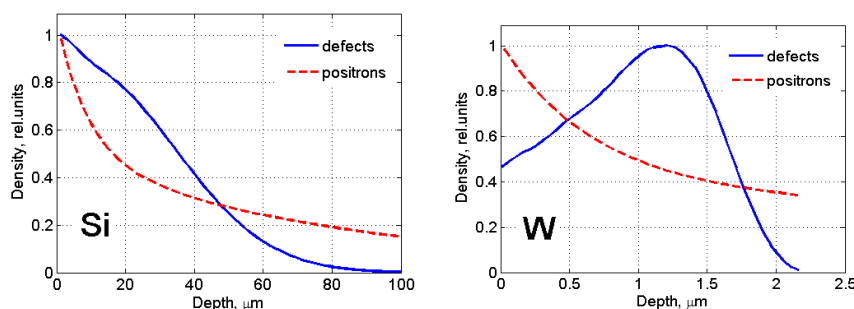


Fig. 1. Positron implantation profiles and Frenkel pairs depth profiles in Si and W samples

In silicon irradiated by protons with energies up to 3 MeV with the fluence $\sim 5 \cdot 10^{14} \text{ cm}^{-2}$, defects are located within 100 μm near-surface region. According to our calculations 72% of positrons annihilate therein. To describe fate of the near-surface positrons we use the standard two-state trapping model. It yields the lifetime of the trapped positrons about 0.3 ns, which indicate that positrons preferentially annihilate in divacancies. Trapping rate is 0.6 ns^{-1} [1]. Using simulated e^+ implantation profile and spatial distribution of radiation defects, we estimated concentration of divacancies in the near-surface region as 10^{17} cm^{-3} .

In the tungsten samples irradiated by W⁶⁺ ions (energy 20 MeV, fluence $1.6 \cdot 10^{12} \text{ cm}^{-2}$) all primary defects ($\sim 0.003 \text{ dpa}$) are located within a 2 μm near-surface layer. Assuming that 27 % of all positrons annihilate therein and the defect concentration $C_d \sim 10^{20} \text{ cm}^{-3}$ exceeds the saturation limit, we determined the lifetime of positrons in the vacancy-type defects as $\tau_d = 0.22 \text{ ns}$, which is essentially higher than lifetime in monovacancies. It indicates the presence of multivacancies.

[1] Dubov L.Yu., Stepanov S.V., Funtikov Yu.V., Shtotsky Yu.V., *Defect and Diffusion Forum*, Vol. 373, pp 209-212 (2016)

**O35 | Combining experiments and theory in positron annihilation techniques:
recent advances and future prospects**

Ilja Makkonen*

*Department of Applied Physics, Aalto University School of Science, P.O. Box 15100,
FI-00076 AALTO, Espoo, Finland*

*email: ilja.makkonen@aalto.fi

The collaboration between positron annihilation experiments and supporting theoretical modeling has been especially fruitful in the identification of vacancy defects in crystalline matter [1] such as semiconductors, metals and alloys. As the structural complexity of the materials systems studied continues to increase, a larger number of defect candidates have to be considered computationally in order to be able to understand trends seen in experiments and the defects or defect complexes are behind the measured data. This is the usually the case in positron studies of complex oxides [2] where cation vacancies are usually complexed with one or more oxygen vacancies, in semiconductor alloys [3] or in multicomponent metallic alloys [4], in which point defects occur in many different atomic configurations. In best cases, thorough experimental work combined with simulations can provide a very detailed picture of the structural and chemical identities of vacancy defects detected [5].

The two-component density functional theory, which is typically the preferred method in defect studies, can quite reliably predict the ground-state of a thermalized positron in a given defect or nanostructure model in solid-state matter. On the other hand, correlated positron states such as surface states are difficult or even impossible to model using existing correlation functionals. In addition to the electron-positron correlation energy and potential, especially the positron annihilation rate and momentum density of annihilation radiation, are difficult to describe in a density-functional formalism.

In this talk, I will discuss some of our past works combining experiment and theory in defect identification. The examples include semiconductors, complex oxides and metallic alloys. I will also discuss some future prospects and ongoing methodological developments. For example, how recent advances of electronic-structure methods could, in principle, be adapted to calculating defect and charge-state-specific trapping rates in semiconductors. Most importantly, I will discuss our preliminary work beyond density-functional theory, namely applying quantum Monte Carlo methods to positrons in condensed matter systems [6].

[1] F. Tuomisto and I. Makkonen, *Reviews of Modern Physics* 85, 1583 (2013).

[2] I. Makkonen, E. Korhonen, V. Prozheeva, and F. Tuomisto, *Journal of Physics: Condensed Matter* 28, 224002 (2016).

[3] V. Prozheeva, I. Makkonen, R. Cuscó, L. Artús, A. Dadgar, F. Plazaola, and F. Tuomisto, *Applied Physics Letters* 110, 132104 (2017).

[4] F. Tuomisto, J. Heikinheimo, I. Makkonen *et al.* (unpublished).

[5] C. Rauch, I. Makkonen and F. Tuomisto, *Physical Review B* 84, 125201 (2011); K. M. Johansen, A. Zubiaga, I. Makkonen, F. Tuomisto, P. T. Neuvonen, K. E. Knutsen, E. V. Monakhov, A. Y. Kuznetsov, and B. G. Svensson, *Physical Review B* 83, 245208 (2011); F. Linez, I. Makkonen and F. Tuomisto, *Physical Review B* 94, 014103 (2016).

[6] K. Simula, I. Makkonen *et al.* (unpublished).

A collimated, energy-tunable positronium beam for the investigation of positronium scattering with surfaces

K. Michishio^{1,2,*}, L. Chiari^{1,3}, F. Tanaka¹, N. Oshima², and Y. Nagashima¹

¹*Department of Physics, Tokyo University of Science, 1-3 Kagurazaka, Shinjuku, Tokyo 162-8601, Japan*

²*National Institute of Advanced Industrial Science and Technology (AIST), 1-1-1 Umezono, Tsukuba, Ibaraki 305-8568, Japan*

³*Department of Applied Chemistry and Biotechnology, Faculty of Engineering, Chiba University, 1-33 Yayoi, Inage, Chiba 263-8522, Japan*

*email: koji.michishio@aist.go.jp

Interactions of positronium (Ps) atoms with materials have long been of interest in research fields, such as atomic and molecular physics, material science and radiation chemistry. When Ps atoms interact with solid surfaces, specular reflection [1] and the spin conversion reaction [2], as well as pick-off annihilation, may take place. If a coherent beam of Ps atoms impinges onto single-crystal surfaces, the diffraction phenomenon of elastically scattered Ps atoms might also occur. This technique might be a unique probing of surface structures owing to the neutrality, lightness and outermost surface sensitivity of Ps [3]. However, because of Ps neutrality and short-lived nature, the production of a Ps beam, that is applicable to surface scattering studies, is very challenging.

In recent years, we have succeeded in the efficient generation of positronium negative ions (Ps⁻), in which an electron is weakly bound to a positronium atom [4]. This technique made it possible to observe its photodetachment [5] and resonant photodetachment [6], and consequently to produce an energy-tunable Ps beam [7]. In the present work, we show the production of a collimated, tunable Ps beam based on a trap-based positron system [8], which can output nano-second positron bursts. Those positron bursts were magnetically guided and focused onto an efficient Ps⁻ converter, a Na-coated W(100) film of 100 nm thick [4]. The Ps⁻ ions emitted from the opposite surface of the film were focused and accelerated by a simple electrostatic lens and then photodetached by a nano-second IR laser pulse to form a Ps beam in the energy range of 200 eV – 3300 eV. In order to reduce the angular divergence, a collimator with a diameter of 1 mm was installed, resulting in a collimated beam with an angular spread of less than 0.1 degrees. This high quality beam can be applied to positronium diffraction experiments with the grazing incidence geometry.

- [1] M. H. Weber *et al.*, *Phys. Rev. Lett.* 61 (22), 2542 (1988).
- [2] C. Dauwe and Mbungu-Tsumbu, *Phys. Rev. B* 45, 9 (1992).
- [3] K. F. Canter, *Positron Scattering in Gases*, p219 (1983).
- [4] Y. Nagashima, *Phys. Rep.* 545, 95–123 (2014).
- [5] K. Michishio *et al.*, *Phys. Rev. Lett.* 106, 153401 (2011).
- [6] K. Michishio *et al.*, *Nature Commun.* 7, 11060 (2016).
- [7] K. Michishio *et al.*, *Appl. Phys. Lett.* 100, 254102 (2012).
- [8] R. G. Greaves and J. Moxom, *AIP Conf. Proc.* 692, 140 (2003).

Studies performed on previous J-PET prototypes

Sz. Niedźwiecki¹ on behalf of J-PET collaboration

¹ *Faculty of Physics, Astronomy and Applied Computer Science, Jagiellonian University,
prof. Stanisława Łojasiewicza 11, 30-348 Kraków*

*email: szymon.niedzwiecki@uj.edu.pl

Assembly of J-PET prototype consisting of 192 detection modules, read out by constant multi-threshold digital electronics, was recently finished at Jagiellonian University. Before its construction two smaller prototypes were developed, build out from 24 and 2 modules [1, 2, 3].

These systems were extensively used for tests of calibration and optimisation techniques as well as development of acquisition system which final version was used in current prototype.

In this presentation a description of performance of first J-PET prototypes will be presented and discussed.

- [1] P. Moskal, Sz. Niedźwiecki et al., *Nuclear Instruments and Methods in Physics Research Section A* 764, 317 (2014)
- [2] L. Raczyński et al., *Physics in Medicine & Biology* 62, 5076 (2017)
- [3] T. Bednarski, PhD Thesis 2016.

Generation of an electrostatically guided Rydberg-Ps beam

D. B. Cassidy*

Department of Physics and Astronomy, University College London, United Kingdom

*email: d.cassidy@ucl.ac.uk

Positronium atoms that have been optically excited to specific Rydberg-Stark states [1] can be used for many experiments that cannot be performed with ground state atoms. This is primarily because the excited states essentially don't annihilate, and will therefore live for times determined by fluorescence (typically microseconds or longer [2]). In addition to having extended lifetimes, Rydberg Ps atoms can also be manipulated using inhomogeneous electric fields owing to their large electric dipole moments [3]. Thus, it is possible to produce a long-lived Ps beam that can in principle be decelerated and focused [4], although so far we have only demonstrated Ps velocity selection, using a curved quadrupole guide [5]. Nevertheless, this configuration is well-suited to the production of merged beams [6], allowing Ps interactions with other atomic and molecular species to be studied. This arrangement would, for example, be ideal for experiments designed to observe the production of positron-atom bound states [7] with very high efficiency, since the relative velocities of the Ps and the atom beam can be made to be low. I will discuss the Rydberg-Ps beam production experiments that have been conducted so far, and consider future prospects and applications.

- [1] *Selective Production of Rydberg-Stark States of Positronium*, T. E. Wall, A. M. Alonso, B. S. Cooper, A. Deller, S. D. Hogan, and D. B. Cassidy, Phys. Rev. Lett. **114**, 173001 (2015).
- [2] *Measurement of Rydberg positronium fluorescence lifetimes*, A. Deller, A. M. Alonso, B. S. Cooper, S. D. Hogan, and D. B. Cassidy, Phys. Rev. A **93**, 062513 (2016).
- [3] *Electrostatically Guided Rydberg Positronium*, A. Deller, A. M. Alonso, B. S. Cooper, S. D. Hogan, and D. B. Cassidy, Phys. Rev. Lett. **117**, 073202 (2016).
- [4] *Rydberg-Stark deceleration of atoms and molecules*, S. D. Hogan, EPJ Tech. Instrum. **3**, 1 (2016).
- [5] *Velocity selection of Rydberg positronium using a curved electrostatic guide*, A. M. Alonso, B. S. Cooper, A. Deller, L. Gurung, S. D. Hogan, and D. B. Cassidy, Phys. Rev. A **95**, 053409 (2017).
- [6] *3D-Printed Beam Splitter for Polar Neutral Molecules*, Sean D. S. Gordon and Andreas Osterwalder, Phys. Rev. Applied **7**, 044022 (2017).
- [7] *Formation of positron-atom bound states in collisions between Rydberg Ps and neutral atoms* A. R. Swann, D. B. Cassidy, A. Deller, and G. F. Gribakin, Phys. Rev. A **93**, 052712 (2016).

O39 | **Recent research and current status of the accelerator based slow positron beam facility at AIST**

Brian E. O'Rourke^{*}, Yoshinori Kobayashi, Wenfeng Mao, Koji Michishio,
Nagayasu Oshima, Ryoichi Suzuki

National Metrology Institute of Japan, National Institute of Advanced Industrial Science and Technology (AIST), 1-1-1 Umezono, Tsukuba, Ibaraki 305-8568, Japan

^{*}email: brian-orourke@aist.go.jp

At AIST, a dedicated electron accelerator is used to produce an intense slow positron beam. This facility is primarily dedicated to materials research via positron annihilation lifetime spectroscopy (PALS). PALS measurements may be performed with unfocussed (~10 mm) or focused (~50-100 μm) variable energy (~1 – 30 keV) pulsed slow positron beams [1]. The focused microbeam uses a single stage transmission type re-moderator and can measure positron lifetimes with a temporal resolution of around 200-300 ps [2]. This microbeam (PPMA: Positron Probe MicroAnalyzer) can be used to perform 1D scans or 2D maps of positron lifetime (and thus defect or free volume size distributions) of the sample [3]. We also have developed techniques to extract the beam into air through a thin vacuum window for achieving PALS in actual environmental condition [4]. Our accelerator based slow positron beamline facility is open to external (both domestic and international) users through the “Nanotechnology Platform” open access program [5].

In addition to our work with slow positron beams, we are also interested in developing techniques for PALS in bulk (~cm sized) samples. To this end, we have performed preliminary experiments using positrons generated inside the sample by high energy photons from a very short pulse length (~ps) S-band electron accelerator [6].

In the presentation we will give an overview of some recent research at our facility and outline some of our plans for further developments.

[1] B. E. O'Rourke *et al.*, *JJAP Conf. Proc.* 2 011304 (2014)

[2] N. Oshima *et al.*, *J. Appl. Phys.* 103 094916 (2008)

[3] N. Oshima *et al.*, *Appl. Phys. Lett.* 94 194104 (2009)

[4] W. Zhou *et al.*, *Appl. Phys. Lett.* 101, 014102 (2012)

[5] <http://nanonet.mext.go.jp/>

[6] Y. Taira *et al.*, *Rad. Phys. Chem.* 95 30 (2013)

Preliminary evaluation of a brightness enhancement system of the KUR slow positron beamline

Yoshihiro Kuzuya^{1,2*}, Nagayasu Oshima², Atsushi Kinomura¹, and Atsushi Yabuuchi¹

¹ Research Reactor Institute, Kyoto University, Osaka 590-0494, Japan

² National Metrology Institute of Japan (NMIJ), National Institute of Advanced Industrial Science and Technology (AIST), Ibaraki 305-8568, Japan

*email: kuzuya.yoshihiro.52e@st.kyoto-u.ac.jp

At present, a reactor-based slow positron beamline, as a part of joint usage research facilities, is under development at the Kyoto University Research Reactor (KUR) [1–4] in order to promote the research on nuclear and other advanced materials using energy-variable slow positron beams. To date, slow positron production tentatively measured was $1.4 \times 10^6 \text{ s}^{-1}$ under 1 MW reactor operation [2] (Maximum 5 MW). The KUR beamline mainly consists of a positron source [2], a brightness enhancement system [3], a pulsing system [4] and an experiment chamber.

A brightness enhancement technique for positron beams has been studied at several facilities for getting high-brightness and low-emittance beams [5, 6]. We use this technique to reduce the beam size from around 30 mm to several mm while keeping the beam intensity as high as possible. Our brightness enhancement system was designed based on the positron microprobe developed at AIST [5] and has been already installed at the beamline. Brightness-enhanced beams are obtained by focusing the accelerated positron beams (5 keV) at the transmission-type remoderator (single-crystal Ni thin film). In our design, the remoderator can be easily retracted from the center of the beamline to adjust the beam transport.

As the KUR has not been in operation for approximately three years (from June, 2014) to comply with new safety regulations, we performed preliminary operation tests by electron beams with respect to the beam extraction from a transport magnetic field and focusing using a magnetic lens. For comparison, we also performed the trajectory analysis of positron beams in the several types of configurations by using GPT [7] and Poisson Superfish [8] codes. In this presentation, we will report the above experimental and calculation results together with the introduction of the recent developments of our slow positron beamline.

This study was financially supported by Innovative Nuclear Research and Development Program of Ministry of Education, Culture, Sports, Science and Technology. We thank all colleagues of Tohoku Univ., Kyoto Univ., KEK, and Tokyo Univ. of Science for their invaluable help.

- [1] Q. Xu et al., J. Phys. Conf. Ser. 505 (2014) 012030.
- [2] K. Sato et al., Nucl. Instr. Meth. Phys. Res. B 342 (2015) 104.
- [3] Y. Kuzuya et al., J. Phys. Conf. Ser. 791 (2017) 012012.
- [4] A. Yabuuchi et al., J. Phys. Conf. Ser. 791 (2017) 012013.
- [5] N. Oshima et al., J. Appl. Phys. 103 (2008) 094916.
- [6] C. Hugenschmidt et al., New J. Phys. 14 (2012) 055027.
- [7] S. B. van der Geer and M. J. de Loos, The General Particle tracer code: Design, implementation and application (2001).
- [8] M. T. Menzel and H. K. Stokes, User's Guide for the POISSON/SUPERFISH Group of codes, Report LA-UR-87-115 (1987), Los Alamos National Lab., New Mexico.

O41 | **Studies of the discrete symmetries in the decays of positronium with J-PET tomograph**

M. Silarski^{1,*} for the J-PET Collaboration

¹*Faculty of Physics, Astronomy and Applied Computer Science, Jagiellonian University,
30-348 Cracow, Poland*

*email: michal.silarski@uj.edu.pl

If the Nature was utterly symmetric the matter would not exist. Yet, processes driven by the gravitational, electromagnetic and strong interactions seem to be symmetric with respect to reflection in space (P), reversal in time (T) and charge conjugation (C). So far violations of these symmetries were observed only in processes governed by the weak interaction. Interestingly, though the matter which we know is made of quarks and leptons, violation of CP and T symmetries have been observed only for systems including quarks, and it has not yet been discovered in any processes involving purely leptonic matter. Positronium is the lightest purely leptonic object decaying into photons. As an atom bound by a central potential, it is a parity eigenstate, and as an atom built out of an electron and an anti-electron, it is an eigenstate of the charge conjugation operator. Therefore, the positronium is a unique laboratory to study discrete symmetries whose precision is limited, in principle, by the effects due to the weak interactions expected at the level of 10^{-14} and photon–photon interactions expected at the level of 10^{-9} . The newly constructed Jagiellonian Positron Emission Tomograph (J-PET) enables to perform tests of discrete symmetries in the leptonic sector via the determination of the expectation values of the discrete-symmetries-odd operators, which may be constructed from the spin of ortho-positronium atom and the momenta and polarization vectors of photons originating from its annihilation. We will present the potential of the J-PET detector to test the C, CP, T and CPT symmetries in the decays of positronium atoms and report on results from the first data-taking campaigns. The J-PET detector, built of plastic scintillators, provides superior time resolution, high granularity, low pile-ups rate, and opportunity of determining photon's polarization. These features allow us to expect a significant improvement in tests of discrete symmetries in decays of positronium atom (a purely leptonic system).

- [1] J-PET: P. Moskal et al., *Acta Phys. Polon. B* 47, 509 (2016)
- [2] J-PET: A. Gajos et al., *Nucl. Instrum. Meth. A* 819, 54 (2016)
- [3] J-PET: D. Kamińska et al., *Eur. Phys. J. C* 76, 445 (2016)
- [4] J-PET: P. Moskal et al., *Phys. Med. Biol.* 61, 2025 (2016)
- [5] J-PET: P. Moskal et al., *Nucl. Instrum. Meth. A* 775, 54 (2015)
- [6] J-PET: P. Moskal et al., *Nucl. Instrum. Meth. A* 764, 317 (2014)
- [7] J-PET: J. Smyrski et al., *Nucl. Instrum. Meth. A* 851, 39 (2017)
- [8] J-PET: L. Raczyński et al., *Phys. Med. Biol.* 62, 5076 (2017)

O42 | **New porosimetric method based on 3g/2g annihilation. Applications to material science and medical imaging**B. Jasińska*Institute of Physics, Maria Curie Skłodowska University, 20-031 Lublin, Poland*

*email: bozena.jasinska@poczta.umcs.lublin.pl

The 3γ fraction determination in positron annihilation is one of the most common analysis of the porous materials. It was successfully applied many times to search materials for experiments containing high porosity targets.

However in the case of the materials containing small free volumes like polymers, annihilation into 3γ is usually neglected, for example in PALS measurements. The attention is paid mainly on the o-Ps lifetime value while the component intensity is less used and rarely interpreted. It is known that in the dense matter, 30-40% of positrons create positronium which can be trapped in free spaces between molecules. There exists correlation between the o-Ps lifetime value τ_{o-Ps} and the free volume size; the larger is volume the longer is the lifetime value. On the other hand it is known that the longer is the lifetime value the larger fraction of ortho-positronium annihilate with emission of three gamma quanta. One can state the fraction of three gamma annihilation reflects free volumes size (lifetime value) and their concentration (intensity value).

The idea of determination of the relative change of the 3γ fraction in the investigated material in comparison to the reference material is proposed. It can be used to follow changes in the porosity of the investigated materials depending on the preparation conditions or measurements temperature, for example.

The proposed idea can be also treated as a keystone to preparation new imaging method during positron emission tomography. PET is a commonly recognized diagnostic method enabling imaging of the metabolism of chosen substances in the living organism. The PET imaging is based on an annihilation of the positron emitted by radiofarmaceutical with an electron from the body of the patient into two gamma quanta with energy of 511 keV each. One of the most important applications is imaging of patients tumour location and size and aiming at the search for the possible metastases as metabolism rate rises significantly in these places and in effect the number of annihilating positrons.

Method proposed here is based on a ratio of three gamma annihilation (from trapped ortho-positronium decay) and two gamma (produced in other processes).

The $f_{3\gamma/2\gamma} = N_{3\gamma}/N_{2\gamma}$ can be determined experimentally as a ratio of the number of 3γ and 2γ events emitted from the patient during PET investigation. It may be used as a measure (morphometric indicator) of the degree of the tissue modification in the investigated organism.

The Pulsed Low Energy Positron System PLEPS: New Developments and Applications to Polymer and Membrane Layers

W. Egger^{1,*}, T. Koschine¹, J. Mitteneder¹, M. Dickmann²,
P. Sperr¹, G. Kögel¹ and G. Dollinger¹

¹*Institut für Angewandte Physik und Messtechnik, Universität der Bundeswehr München,
Werner-Heisenberg-Weg 39, 85577 Neubiberg, Germany*

²*FRM2, MLZ, Lichtenbergstraße 1, 85748 Garching, Germany*

*email: werner.egger@unibw.de

The pulsed low energy positron system PLEPS [1] is a user facility for defect depth-profiling with positron lifetime measurements using a monochromatic pulsed positron 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 count-rates between 5000-10000 counts per second, depending on the sample. It takes typically about 10 minutes for a lifetime spectrum with more than 3×10^6 counts at a single energy. A full depth-profile with 10-15 energies requires about 2-4 hours. Depending on the detector, an overall time-resolution of 220 ps-280 ps and peak-to-background ratios of up to 1×10^5 can be routinely achieved with 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.

Besides defect identification in thin layers and layered structures of semiconductors, insulators, irradiated materials typical applications of PLEPS comprise also the characterization of open volumes in glasses [4], polymers, polymer- and membrane layers [5].

In this talk we will describe the present setup of PLEPS and its performance, show some exemplary applications in the field of polymers, polymer and membrane layers and give an outlook of new developments.

[1] W. Egger, in *Proceedings of the International School of Physics "Enrico Fermi", Course CLXXIV* (eds. A. Dupasquier and A. P. Mills jr.), IOS Press: Amsterdam, 419 (2010).

[2] Ch. Hugenschmidt, and C. Piochacz, *J. large scale research facilities JLSRF* 1, A 22 (2015).

[3] W. Egger, *J. large scale research facilities JLSRF* 1, A 25 (2015).

[4] T. Koschine *et al.*, *J. Polym. Sci. Part B* 53, 213 (2015).

[5] M. Zanatta *et al.*, *Phys. Rev. Lett.* 112, 045501 (2014).

O44 | **Two-component density functional study of positron-vacancy interaction in metals and semiconductors**

S. Ishibashi*

*Research Center for Computational Design of Advanced Functional Materials (CD-FMat),
AIST, 1-1-1 Umezono, Tsukuba, Ibaraki 305-8568, Japan*

*email: shoji.ishibashi@aist.go.jp

The positron can be utilized as a powerful probe for detecting vacancy-type defects in various solids, since positrons are selectively trapped there [1,2]. Theoretical calculations are often crucial in interpreting experimental results and in identifying defect species. To describe the positron state in solids, where many nuclei and electrons exist, Boroński and Nieminen proposed the two-component density-functional-theory formalism [3]. In many practical calculations, a simplification is made assuming that the positron affects neither the electronic structure nor the atomic arrangement. This simplified scheme is called “conventional scheme”. So far, there have been a limited number of applications of the two-component scheme in calculating positron states trapped at defects. One reason is that the computational cost for the two-component scheme is approximately 10 times higher than that for the conventional scheme. Another reason is that, in many cases, the conventional scheme and the two-component scheme give similar annihilation parameters (Doppler broadening spectra and positron lifetimes) because of the feedback effect [4]. We calculated Doppler-broadening spectra and positron lifetimes using the two schemes for divacancies in C, Si, Ge, SiC, AlN, GaN and InN and found that the difference between the two schemes depends on the bulk modulus [5]. For the relatively soft materials Si and Ge, the difference is significant.

In this study, the positron-vacancy interaction has been investigated systematically in d-block metals (except for Mn, Tc, and Hg) [6], Mg and Al as well as in III-V and II-VI semiconductors. Positron states and lifetimes for (cation) vacancies in these metals and semiconductors have been calculated by the conventional (CV) scheme and the two-component (TC) scheme with and without atomic-position relaxation. As an example of the results, the degree of atomic-position relaxation around the vacancy for metals is shown in Fig. 1.

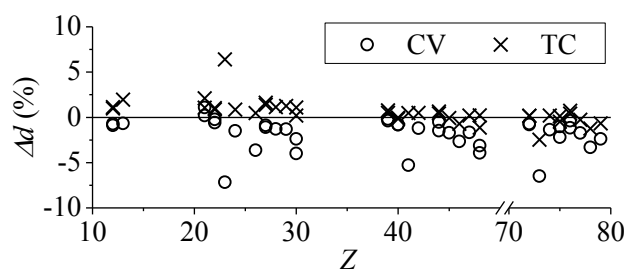


Fig.1. Z (atomic number)-dependence of the change in average distance Δd of the nearest-neighbor atoms from the vacancy center after atomic-position relaxation

- [1] M. J. Puska and R. M. Nieminen, *Rev. Mod. Phys.* **66**, 841 (1994)
- [2] F. Tuomisto and I. Makkonen, *Rev. Mod. Phys.* **85**, 1583 (2013).
- [3] E. Boroński and R. M. Nieminen, *Phys. Rev. B* **34**, 3820 (1986)
- [4] M. J. Puska, A. P. Seitsonen and R. M. Nieminen, *Phys. Rev. B* **52**, 10947 (1995)
- [5] S. Ishibashi and A. Uedono, *J. Phys.: Conf. Ser.* **674**, 012020 (2016)
- [6] S. Ishibashi, *J. Phys. Soc. Jpn.* **84**, 083703 (2015)

Hydrogen interaction with vacancies in Ti

P. Hruška^{1,*}, J. Čížek¹, J. Knapp¹, O. Melikhova¹, L. Havela¹, S. Mašková¹ and F. Lukáč²

¹Faculty of Mathematics and Physics, Charles University,
V Holešovičkách 2, 18000, Praha 8, Czech Republic

²Institute of Plasma Physics of the Czech Academy of Sciences,
Za Slovankou 1782/3, 182 00 Prague 8, Czech Republic

*email: peta.hruska.l@gmail.com

Titanium is an exothermic absorber of hydrogen. In the hydride phase Ti is able to absorb the hydrogen concentration as high as 1.4 wt.%. These properties make Ti and Ti-based alloys attractive for hydrogen storage applications. Hydrogen absorbed in Ti lattice may be trapped at open volume defects like vacancies, dislocations or grain boundaries. Hydrogen is not only trapped at existing defects but new defects can be also introduced by hydrogen loading. For these reasons it is very important to investigate interaction of hydrogen with defects in Ti.

In the present work hydrogen interaction with vacancies and vacancy-like defects in Ti was investigated employing positron lifetime spectroscopy combined with *ab-initio* theoretical modeling of vacancy hydrogen complexes.

Ab-initio modeling revealed that multiple hydrogen atoms can be trapped at vacancies in α -Ti lattice. In the lowest energy configuration hydrogen atoms are located close to the nearest neighbor tetrahedral sites around vacancy, see Fig. 1a. Lifetimes of positrons trapped at vacancies surrounded by various number of hydrogen atoms were calculated and are plotted in Fig. 1b. The equilibrium concentration of vacancy–hydrogen complexes has been calculated as well.

Positron lifetime measurement revealed that phase transition into the hydride phase is always accompanied by introduction of dislocations. Vacancies are created by hydrogen loading as well and agglomerate into small vacancy clusters. Absorbed hydrogen segregates at inner surfaces of these vacancy clusters.

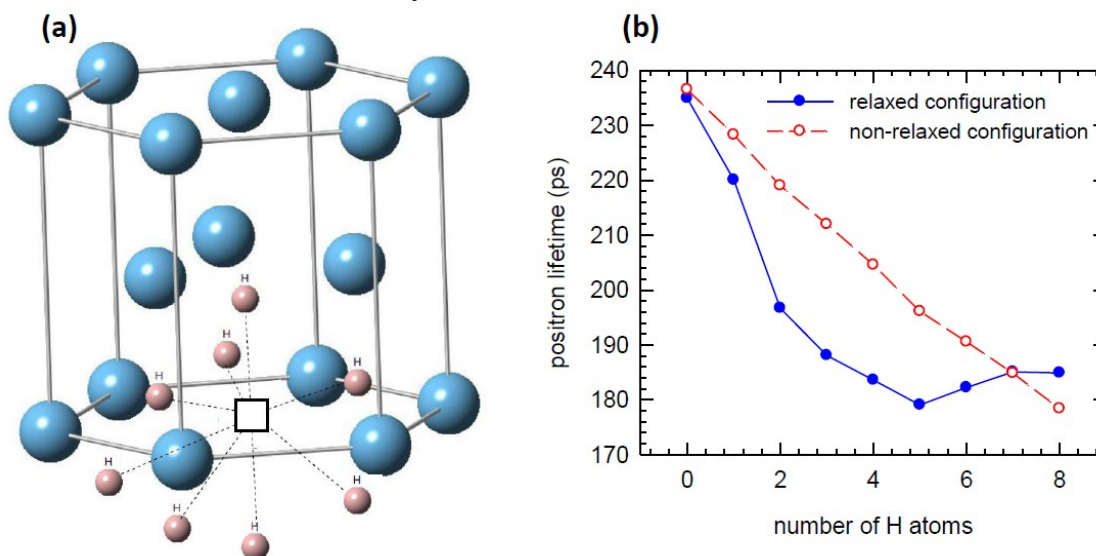


Fig.1. (a) Schematic depiction of a vacancy surrounded by 8 hydrogen atoms in the nearest neighbor tetrahedral sites; (b) calculated lifetimes of positrons trapped at vacancies surrounded by various numbers of hydrogen atoms.

O46 | **Positron probing of open vacancy volume of a thermally stable phosphorus-vacancy complex in electron-irradiated silicon**

N.Yu. Arutyunov^{1, 2, 4, *}, V.V. Emtsev², M. Elsayed¹, R. Krause-Rehberg¹,
N. Abrosimov⁵, G.A. Oganessian² and V.V. Kozlovski³

¹*Department of Physics, Martin Luther University, 06120 Halle, Germany*

²*Ioffe Physico-Technical Institute, 194021 St. Petersburg, Russia*

³*St. Petersburg State Polytechnical University, 195251 St. Petersburg, Russia*

⁴*Institute of Electronics, 700170 Tashkent, Uzbekistan*

⁵*Leibniz-Institute for Crystal Growth, D-12489 Berlin, Germany*

*email: n_arutyunov@yahoo.com

We will discuss theoretical and experimental data related to a microstructure of the phosphorus-vacancy complex which has been elusive from observation for decades in float zone silicon single crystals, n-FZ-Si(P). A surprising behaviour of the positron lifetime was investigated in the course of annealing of material irradiated by 0.9-MeV electrons. It turns out that a well-known procedure of isochronal annealing of irradiated wafers for restoring the electrical activity of the phosphorus dopant by decomposing the phosphorus-vacancy pairs of radiation origin (so-called E-centers) is far from perfection: a considerable amount of the impurity atoms of phosphorus are remaining inactive as the shallow donors in the course of isochronal annealing from ~ 100 °C to ~ 175 °C. A new approach is needed because much higher annealing temperatures are required for restoring electrical parameters of the irradiated material which is of paramount importance for the semiconductor technology.

To gain insight into microstructure of thermally stable radiation centers suppressing electrical activity of the phosphorus dopant we have investigated their isochronal annealing.

The decomposing of these centers was found to begin at ~ 300 °C [1]. The defect-related long positron lifetime $\tau_2 \sim 278$ ps is steady up to the limit of its reliable detecting at the annealing temperature ~ 500 °C; the average positron lifetime τ_{av} just approaches to the value 216 ps characteristic of the non-irradiated material.

These data correlate with the ones of low-temperature Hall effect measurements demonstrating for the same material that the isochronal annealing is complex. Three stages were found for recovery of the concentration of charge carriers and mobility [2]: ~ 100 °C – 180 °C, ~ 200 °C – 300 °C, and at ~ 600 °C – 650 °C the annealing is accomplished.

It is argued that the thermally stable defects are the phosphorus-vacancy complexes, P- V_{op} . The open vacancy volume V_{op} to be characterized by long positron lifetime $\tau_2 \sim 278$ ps in P- V_{op} complex is compared with theoretical data available for the vacancies and divacancies.

The extended semi-vacancies, $2V_{s-ext}$, and relaxed vacancies, $2V_{inw}$, are proposed as the open volume V_{op} . It is suggested that larger number of P-Si bonds (at least, five; PSi_5) in the microstructure V_{s-ext} -P- V_{s-ext} underlies its high thermal stability. In this case the open volume V_{op} is equal to $2V_{s-ext}$ and V_{s-ext} -P- V_{s-ext} complex possesses a distorted D_{3d} (or O_h) symmetry. In the light these data, a necessity of reconsideration of the whole conception of formation of the positron-sensitive phosphorus-vacancy complexes in silicon is shortly discussed.

[1] N. Arutyunov, V. Emtsev, R. Krause-Rehberg, M. Elsayed, G. Oganessian, and V. Kozlovski, *Phys. Stat. Sol. (c)*, 13, 807 (2016)

[2] V.V. Emtsev, N.V. Abrosimov, V.V. Kozlovski, G.A. Oganessian, and D.S. Poloskin, *Semiconductors* 50, 1291 (2016).@ Pleiades Publishing Ltd., 2016

Potential of the J-PET tomograph for multi-photon medical imaging

M. Moskal^{1,*} for the J-PET Collaboration

¹*Faculty of Physics, Astronomy and Applied Computer Science, Jagiellonian University,
30-348 Cracow, Poland*

*email: p.moskal@uj.edu.pl

The Jagiellonian Positron Emission Tomograph (J-PET) is the first PET built from plastic scintillators. J-PET prototype consists of 192 detection modules arranged axially in three layers forming a cylindrical diagnostic chamber with the inner diameter of 85 cm and the axial field-of-view of 50 cm. An axial arrangement of long strips of plastic scintillators, their small light attenuation, superior timing properties, and relative ease of the increase of the axial field-of-view opens promising perspectives for the cost effective construction of the whole-body PET scanner, as well as construction of MR and CT compatible PET inserts. Present status of the development of the J-PET tomograph and its possibilities for multi-photon and positronium imaging will be presented and discussed.

- [1] J-PET: P. Moskal et al., *Nucl. Instrum. Meth. A* 764, 317 (2014)
- [2] J-PET: P. Moskal et al., *Nucl. Instrum. Meth. A* 775, 54 (2015)
- [3] J-PET: P. Moskal et al., *Acta Phys. Polon. B* 47, 509 (2016)
- [4] J-PET: A. Gajos et al., *Nucl. Instrum. Meth. A* 819, 54 (2016)
- [5] J-PET: D. Kamińska et al., *Eur. Phys. J. C* 76, 445 (2016)
- [6] J-PET: P. Moskal et al., *Phys. Med. Biol.* 61, 2025 (2016)
- [7] J-PET: J. Smyrski et al., *Nucl. Instrum. Meth. A* 851, 39 (2017)
- [8] J-PET: L. Raczyński et al., *Phys. Med. Biol.* 62, 5076 (2017)

O48 | Advanced positron techniques for practical applications: history, current, and future developments

F.A. Selim

Department of Physics and Astronomy, Bowling Green State University, Ohio 43403, USA
Center for Photochemical Sciences, Bowling Green State University, Ohio 43403, USA

email: faselim@bgsu.edu

Positron annihilation spectroscopy (PAS) is often performed using radioactive sources for bulk measurements or positron beams for depth resolved measurements. Both have many advantages and great capabilities for a variety of applications. In the recent history, we have shown that PAS can be also carried out directly using high energy photons without creating positron source or positron beams [1,2]. This approach brings unique capabilities for some specific applications and promotes the use of PAS in new areas of materials science and probably in industrial applications. Some of the important applications include developing new nondestructive highly penetrating sensitive probe for structural and engineering materials. I will present some data to support this claim. It can also greatly advance the applications of PAS in semiconductors, electronic and photonic materials as well as in polymers, ceramics and liquids. The recently developed Gamma induced positron spectroscopy (GIPS) [3,4] in HZDR in Dresden provides a state of the facility for many of these applications [5].

It In this talk, I will present the history and development of the technique, the current and future facilities. A facility for this technique can be easily incorporated in a wide range of accelerators and nuclear reactors at modest cost. I will show examples for that including the use of table top electron accelerators and Van De Graff accelerators and present a concept and design for its incorporation in a small research nuclear reactor.

When incorporated with pulsed accelerators, this technique may trigger novel studies of transient states in matter and explore several solid-state processes that take place on short time scale [6].

- [1] F. A. Selim, D.P. Wells., J. F. Harmon, and J. Williams, *Journal of Applied Physics* 97, 113539 (2005).
- [2] F. A. Selim, D.P. Wells., J. F. Harmon, *Review Scientific. Instruments.* 76, 033905 (2005)
- [3] A. Wagner et al., *Journal of Physics: Conference Series* 618, 012042 (2015).
- [4] A. Wagner et al., *Defect Diff. Forum.* 331, 41-52 (2012).
- [5] J. Ji et al, *Scientific Reports* 6, 31238, 2016.
- [6] F. A. Selim, *Physics Letters A* 344, p. 291, 2005.

Online Processing of Tomographic Data

G. Korcyl^{1,*}

¹*Department of Information Technologies, Jagiellonian University, Łojasiewicza 11, 30-348
Kraków, Poland*

*email: grzegorz.korcyl@uj.edu.pl

Abstracts

poster presentations

P1 | **Application of the theory of excitons to study of the positronium in matter.
Optical transition during positronium formation in matter**

M. Pietrow*

*Institute of Physics, M. Curie-Skłodowska University, ul. Pl. M. Curie-Skłodowskiej 1, 20-031
Lublin, Poland*

*email: mrk@kft.umcs.lublin.pl

Considerable similarity between a positronium atom (Ps) in matter and an exciton in a quantum dot is indicated. Following this, we apply the calculation regime from the theory of excitons to describe some aspects of formation of a Ps in matter. We consider the possibility of photonic deexcitation during Ps formation and show the way of calculation of its probability.

The photonic transitions speculated here, if detected, allows improving experimental studies of solid matter with positron techniques.

P2 | **Positron interactions with natural and synthetic chiral quartz crystals in non-z orientations**

 F. Wu*, Y.C. Jean and J.D. Van Horn

Chemistry Department, University of Missouri–Kansas City, 5110 Rockhill Road, Kansas City, Missouri 64110, USA

*email: fww77@mail.umkc.edu

The interactions of energy and particles in asymmetric substances has been of fundamental research interest since the discovery of chirality [1]. A well-studied asymmetric crystalline material is α -quartz [2], which has a helical structure associated with its crystallographic z-axis. Previously, we reported a large difference in ‘free positron’ annihilation lifetime and intensity between samples of LH and RH quartz single crystals [3]. In the current project, we investigated natural versus synthetic quartz in z and non-z orientations using PALS to confirm asymmetric interactions and to compare different orientations. As before, we observed significant lifetime and intensity differences in free positronium annihilation for LH and RH quartz crystals (Figure 1). The trend was also found to be the same for the similar crystallographic orientations of LH or RH crystals; that is, the direction of incident positrons, z or non-z, did not affect the observed differences in lifetime and intensity trends. The results are attributed to differential interactions of positronium with the asymmetric lattice structures of LH and RH quartz. This result may point to the positron or positronium species being sensitive to the small electroweak energy difference between enantiomers [4]. Further, the results may be considered an example of particle stereo-recognition.

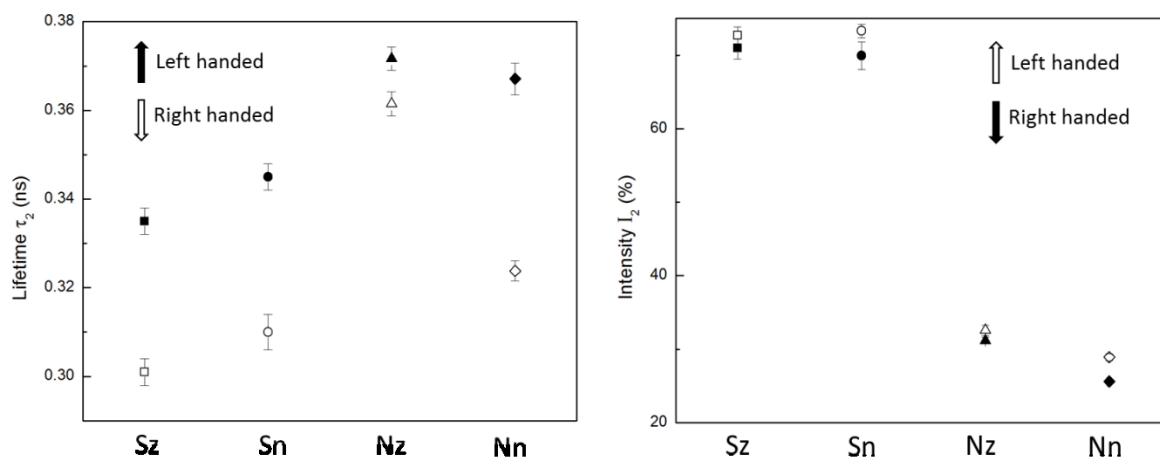


Fig.1. Lifetime and intensity differences in ‘free positron’ annihilation for LH and RH chiral crystals. S / N / z / n represent synthetic and natural quartz, and the z and non-z crystal orientations, respectively.

- [1] L. Pasteur, *CR Hebd. Acad. Sci.*, **26**, 535 (1848).
- [2] H. Saito and T. Hyodo, *Phys. Rev. Lett.*, **90**, 19 (2003).
- [3] J.D. Van Horn, F. Wu, G. Corsiglia and Y.C. Jean, *Def. Diffus. Forum*, **373**, 221 (2016).
- [4] R. Bast, et al., *Phys. Chem. Chem. Phys.*, **13**, 865 (2011).

P3 | **The POCOBIO database: a database for computed scattering cross sections for positron collisions with biomolecular systems**

J. Franz

Department of Theoretical Physics and Quantum Informatics, Faculty of Applied Physics and Mathematics, Gdansk University of Technology, ul. Narutowicza 11/12, PL 80-233 Gdansk, Poland

* email: jfranz@mif.pg.gda.pl

The design of a database for positron interactions with biomolecular systems is outlined. The database contains only scattering cross sections, which are derived from theory. The data model is defined in a very flexible way, which facilitates its usage as a repository for weakly bound clusters of molecules and molecular systems with many tautomeric forms. one empty line.

The focus on theoretical data allows to have a consistent set of data. The database should fulfill following purposes:

- work as a repository for cross section data,
- allow easy access to published data so, that the data can be used in computer program packages for simulation of positron tracks,
- provide benchmark data for other calculations and for experimentalists,
- and provide differential cross sections, which allow experimentalists to correct experimentally obtained integral cross sections.

P4 | **Positron annihilation lifetime spectroscopy of ABS objects manufactured by fused deposition modelling**

M. Dryzek¹, E. Dryzek^{2,*}

¹*Institute for Computational Civil Engineering, Cracow University of Technology, Krakow, Poland*

²*Institute of Nuclear Physics Polish Academy of Sciences, PL-31342 Kraków, Poland*

*email: ewa.dryzek@ifj.edu.pl

The mechanical properties of acrylonitrile butadiene styrene (ABS) objects manufactured using fused deposition modelling is subject of many studies due to the growth in popularity of this method of production. The most noticeable property of the material is its anisotropy of the mechanical behaviour caused mainly by introduction of voids throughout production process but also by different properties of filament build surfaces and weld interfaces. The recent studies suggest that the difference may result from various molecular structures of the build and the interface which occurs for different build orientation [1].

In the research ABS specimens were subjected to positron annihilation lifetime spectroscopy (PALS) to explore possibilities of identifying differences in molecular structure inside the material. The set of specimens was prepared including square tiles and long rectangular tiles with all filament beads parallel to longer edge. Both types of tiles were produced with various filament overlapping parameter with overlapping both in horizontal and vertical direction. The results show that despite different overlapping parameters changes of the PALS parameters are small especially within the same specimen shape.

[1] D. P. Cole, J. C. Riddick, H. M. Iftexhar Jaim, K. E. Strawhecker, N. E. Zander, Appl. Polym. Sci. 133 (2016) DOI: 10.1002/APP.43671

Free-volume and mechanical properties of glass fibre reinforced polyamide 6 composites

E. Dryzek^{1,*}, M. Wróbel² and E. Juszyńska-Gałązka¹

¹*Institute of Nuclear Physics Polish Academy of Sciences, PL-31342 Kraków, Poland*

²*AGH University of Science and Technology, 30 Av. Mickiewicza, 30-059 Kraków, Poland*

*email: ewa.dryzek@ifj.edu.pl

Increasing demands connected to various technological applications of polymer materials result in development of polymer composites reinforced with inorganic fillers. Polyamide is one of the basic engineering polymer materials. Its mechanical properties can be easily modified by using suitable fillers.

The external load in such heterogeneous polymer systems causes micromechanical deformation processes determined to a large extent by the properties of the matrix polymer. One of the factors taken into account while considering the mechanisms of inelastic deformation in amorphous polymers is free volume. The volume excess is an important factor that enables local shear transformations [1,2]. On the other hand local free volume properties of the material can be determined directly by positron annihilation lifetime spectroscopy (PALS).

The materials investigated in this study were polyamide 6 and polyamide 6 composites with 15 and 30% of glass fibre, i.e., ArtAMID6 15GF and ArtAMID6 430GF. The tensile tests were performed for the paddle shaped specimens injection moulded in accordance with the appropriate standards. The test allowed us to obtain the stress-strain curves and determine the tensile properties of the samples. The positron lifetime measurements were performed for the as received samples and for the samples in the vicinity of the break after they failed. Local free volume size exhibited some distribution which was initially narrower for the composite samples in comparison to the polyamide 6 sample and became broader as a result of the deformation. This indicates that after deformation actual sizes of the local free volume are scattered over a broader range of radii in spite of the small changes of their mean size. The deformation caused also increase of the ortho-positronium intensity in the obtained positron lifetime spectra.

[1] A.S. Argon, V.V. Butalov, P.H. Mott, U.W. Suter, *J Rheol*, **39**, 377 (1995).

[2] S. Goyanes, G. Rubiolo, W. Salgueiro, A. Somoza, *Polymer* **46**, 9081 (2005).

Extraction of chemical information using positron annihilation spectroscopy in metal-chitosan complex

X. Z. Cao^{1,*}, R. Xia¹, J. Yang^a, M. F. Zeng², B. Y. Wang¹ and L. Wei¹

¹*Institute of High Energy Physics, Chinese Academy of Sciences, 100049 Beijing, China*

²*Zhejiang Key Laboratory of Alternative Technologies for Fine Chemicals Process, Shaoxing University, Shaoxing 312000, China*

*caoxzh@ihep.ac.cn

The importance of functional polymeric material considering its properties at the molecular level has been attracting increasing attention in materials science. As an intuitive theoretical concept, the free volume has been widely used to explain the physicochemical or macroscopic properties correlated with molecular level of polymer [1]. Positron annihilation spectroscopy (PAS) was proved to be successful in characterizing for free-volume hole properties. Considering that free volume properties, e.g., free-volume hole size and concentration, of polymer can be well correlated with the detected orthopositronium (o-Ps) annihilation information (lifetime and intensity), of essential importance for the development of molecular insights is a better understanding of positron annihilation physical essence or characteristics in polymeric system with complex chemical environment [2,3].

Our previous studies of addition of chloride salt ions coordinated with chitosan molecular chains confirmed the chemical inhibition effect on positronium formation [4]. In the present work, we investigate the effect of three kind of anions existed in polymer matrix on positron annihilation characteristics. A combined use of positron annihilation lifetime spectroscopy (PALS) and Coincidence Doppler broadening (CDB) spectroscopy to illustrate how anions, including chloride ion, nitrate ion and acetate ion, coordinated in molecular chains influence the annihilation of thermalized positrons in chitosan matrix

Acknowledgements

This work is supported by National Natural Science Foundation of China (11475197 and 11575205).

- [1] G. S. Grest and M. H. Cohen, *Phys. Rev. B* 21, 4113 (1980)
- [2] Kobayashi and Y. Zheng, *Macromolecules* 22, 2302 (1989)
- [3] Zubiaga, A and Garcia, J. A. *Phys. Rev. B* 75, 205305 (2007)
- [4] R. Xia and X. Z. Cao, *Phys. Chem. Chem. Phys.* 19, 3616 (2017)

P7 | Study on the surface microstructure of the aged silicone rubber composite insulators by PALSZheng Wang, Feng Zheng, Chunqing He, Pengfei Fang**Key Laboratory of Nuclear Solid Physics Hubei Province, School of Physics and Technology, Wuhan University, Wuhan 430072, China*

*email: fangpf@whu.edu.cn

The silicone rubber composite insulators are being increasingly used instead of porcelain or glass for outdoor insulation application. In this paper, the variations in surface microstructure of polydimethylsiloxane (PDMS) elastomers after argon plasma treating for different time have been investigated by X-ray photoelectron spectroscopy (XPS), slow positron beam and scanning electron microscope (SEM). Inorganic silica-like layer was probed by XPS, after 3 min or longer time of treatments. By using slow positron beam, the thicknesses of silica-like layer for 3 min, 5 min, and 10 min aged samples were estimated as 26 nm, 28 nm and 80 nm, respectively. Among these 3 min and 5 min treated samples, the peak height in S(E) curve increased, indicating the accumulation of low molecular weighted (LMW) siloxanes beneath silica-like layer due to its blocking effect. However, the S(E) curve peak height of 10 min treated sample decreased dramatically. The result suggested that the silica-like layer cracked after long time of plasma treatment, and LMW oligomers diffused through these cracks. SEM images revealed that inorganic fillers were also exposed after 10 min of treatment, indicating the removing of polymeric sample surface. Then the silica-like layer grows thicker. Whereas, short time (≤ 3 min) argon plasma treatments can only remove surface preexisting LMW siloxanes and induce a few PDMS chain scission reactions on the sample surface.

This work was financially supported by the National Natural Science Foundation of China (No. 21174108), the Science and Technology Project of China Southern Power Grid Co., Ltd. (K-GD2014-185).

- [1] B. Larson, et al., *Langmuir* 29, 12990 (2013).
- [2] A. Tóth, et al. *J. Appl. Polym. Sci.* 52, 1293 (1994).
- [3] P. Mallona, et al., *Radiat. Phys. Chem.* 68, 453(2003).
- [4] C. He, et al., *J. Chem. Phys.* 122, 214907 (2005).
- [5] Y. Zhu, et al., *Polym. Degrad. Stab.* 91, 1448 (2006).
- [6] F. Zheng, et al., *Appl. Surf. Sci.* 283, 327 (2013).
- [7] H. Hillborg, et al., *Polymer*. 42, 7349 (2001).

Thermal development of free volumes in Nafion membrane

O. Melikhova^{1,*}, J. Čížek¹, L. Košinová¹, P. Hruška¹

¹*Faculty of Mathematics and Physics, Charles University,
V Holešovičkách 2, 18000, Praha 8, Czech Republic*

*email: Oksana.Melikhova@mff.cuni.cz

Nafion is perfluorosulfonated cation exchange membrane developed by du Pont de Nemours & Co. Inc. Nafion exhibits a high proton conductivity and excellent thermal and chemical stability. These properties make Nafion very attractive for applications in fuel cells and gas separation processes. Nafion exhibits mesoscopic structure consisting of hydrophobic polytetrafluoroethylene (PTFE) skeleton and hydrophilic ionic clusters.

Gas transport through Nafion membrane is controlled by the morphology and size distribution of nanoscopic free volume holes providing suitable pathways. This makes characterization of free volume holes in Nafion extremely important. Ortho-positronium (o-Ps) is a unique probe of nanoscopic free volume holes due to pick-off annihilation process which makes the o-Ps lifetime sensitive on the size of free volume hole where o-Ps is confined.

In this work we employed positron lifetime spectroscopy for investigation of the thermal development of free volumes in Nafion over a broad range of temperatures from -150 to 150°C. Positron lifetime studies were combined with differential scanning calorimetry.

Our investigations revealed that the mean size of free volumes strongly increases with temperature. Two transition temperatures corresponding to a change in the slope of the temperature dependence of o-Ps lifetimes τ_{o-Ps} were identified, see Fig. 1a. The width of the size distribution of free volumes increases with temperature as well, see Fig. 1b. On the other hand, the Ps yield decreases with temperature as shown in Fig. 1c. Results of positron lifetime spectroscopy agree well with the curves obtained by differential scanning calorimetry.

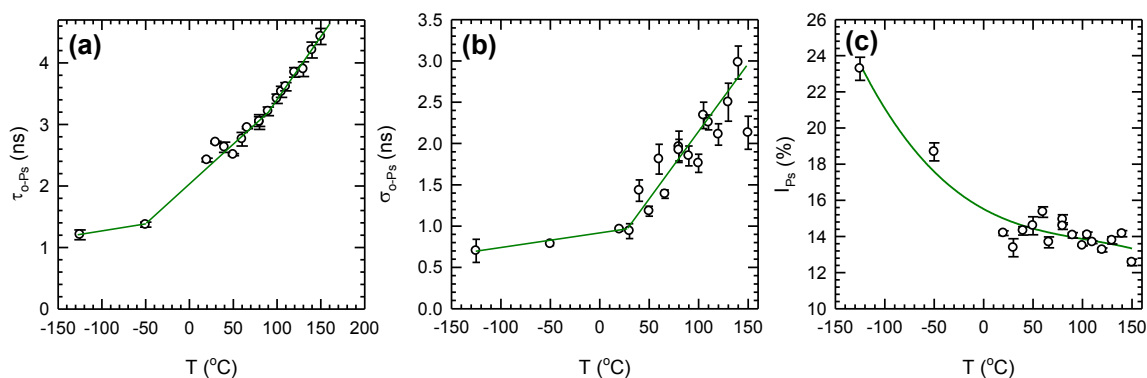


Fig.1. Temperature dependence of (a) the mean o-Ps lifetime τ_{o-Ps} ; the width (one standard deviation) σ_{o-Ps} of the size distribution of free volumes; (c) the intensity of the Ps contribution in positron lifetime spectra.

P9 | **Microstructure characterization of Nafion HP JP as a proton exchange membrane for fuel cell: positron annihilation study**

Hamdy F.M. Mohamed^{1, 2*}, E.E. Abdel-Hady¹, M.O. Abdel-Hamed¹ and Michael Said¹.

¹*Physics Department, Faculty of Science, Minia University, P.O Box 61519 Minia, Egypt*

²*Renewable Energy Science & Engineering Department, Faculty of Postgraduate Studies for Advanced Science (PSAS), Beni-Suef University, P.O. Box 62511 Beni-Suef, Egypt*

*e-mail: hamdyfm@gmail.com

Proton exchange membrane fuel cell (PEMFC) achieves a potential success as an alternative energy source due to its direct electricity conversion, being environmentally friendly and high efficiency. The improvement of an efficient PEMFC strongly depends on the development of a polymer electrolyte membrane (PEM) with high proton conductivity, low fuel cross-over and low cost. Positron annihilation lifetime spectroscopy (PALS) can describe the internal microstructure of the material. In PEM, free volume strongly affects membrane characteristics such as proton conductivity and fuel crossover. In this work, the variation of the free volume of Nafion HP JP membrane was investigated at a wide range of temperature and relative humidity. The influence of temperature and relative humidity on the microstructure of the membrane under study was detected by studying the variation of the o-Ps lifetime τ_3 and its intensity I_3 . It was found that increasing temperature of the sample increases the value of τ_3 as a result of thermal expansion. Phase transition occurred from the glassy state to the rubbery state at glass transition temperature. The crystal structure and thermal stability were compared before and after heat treatment by wide angle x-ray diffraction and thermo gravimetric analysis, respectively. On the other hand, the effect of relative humidity up to 80% on the free volume has been also studied by PALS technique using a specially designed chamber and accurately controlled humidity system. A correlation between data obtained from PALS and proton conductivity measurement was successfully achieved. All the previous measurements were carried out under the same conditions to the standard Nafion NRE212 for comparison.

Free volume in strained rubber with carbon black filler by positron annihilation spectroscopy

M. Nippa^{1,*}, Y. Ikeda², A. Kato³, A. Komatsu¹, L. Chiari¹ and M. Fujinami¹

¹*Department of Applied Chemistry, Chiba University, 1-33 Inage, Yayoi 263-8522, Japan*

²*Kyoto Institute of Technology, Matsugasaki, Kyoto 606-8585, Japan*

³*NISSAN ARC, LTD., Natsushima 1, Yokosuka, Kanagawa 237-0061, Japan*

*email: madoka.nippa@chiba-u.jp

The main component of tires is natural rubber, and various additives are added to increase the strength of the rubber. Carbon black (CB), which is dispersed in the rubber, is known to remarkably improve its mechanical properties. This reinforcing effect is thought to be related to the CB network, in which CB particles are connected to each other within a 3-nm thick layer, the so-called bound rubber, at the CB/rubber interface [1]. However, the detailed reinforcement mechanism is still unknown. In this study, we aimed to investigate the mobility of molecular chains in rubber by measuring the change in free volume within strained rubber with various amounts of carbon black filler by positron annihilation spectroscopy.

The rubber consisted of isoprene rubber (IR) filled with various amount of CB (N330). The rubber specimens were prepared by mixing IR, CB and 1 phr (phr: parts by weight per 100 parts by weight of rubber) DCP (dicumyl peroxide) as the crosslinking agent. The CB content was varied from 0 to 80 phr. The rubber samples were strained to a ratio of 160% with a tensile tester and several consecutive positron lifetime measurements were carried out in situ for about 100 hours in total. After releasing the samples, they were measured once again.

The o-Ps lifetime dependence on the CB content is shown in Fig.1. The o-Ps lifetime showed a minimum at 40 phr and generally no large changes were observed. The results shown in Fig. 1 were very similar to the dependence of the branch chain fraction of the CB network structure (number of branched chains / (number of branched chains + number of crosslinked chains)) on the CB content [1]. Afterwards, the o-Ps lifetime of the strained samples measured in situ. The o-Ps lifetime of the rubber samples hardly changed with and without strain. On the other hand, a decrease in the intensity of the o-Ps component was observed in the strained samples and the maximum decrease of 3 % was measured in the sample containing 40 phr CB. After releasing the sample, the intensity recovered. It is believed that the molecular chains in the amorphous phase become aligned when subject to tensile stress, thus leading to a decrease in Ps formation.

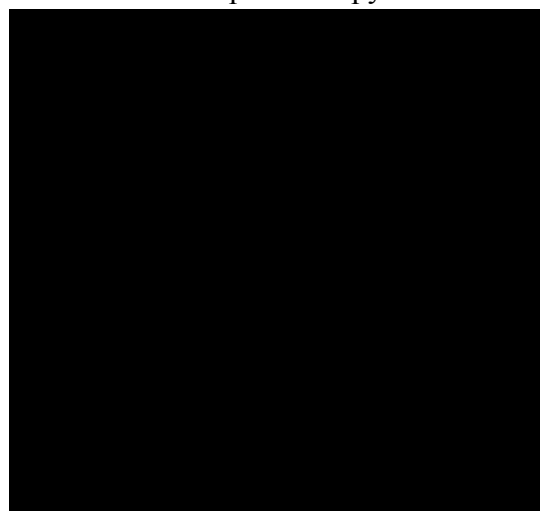


Fig.1. o-Ps lifetime dependence of CB content

[1] A. Kato *et al.*, *Japan Rubber Association Magazine* 87, 447 (2014).

P11 | **Nano-porosity of polymeric sorbents and membrane materials as seen by PALS and low temperature gas sorption**

V.P. Shantarovich^{1,*}, V.G. Bekeshev¹, I.B. Kevdina¹, Yu.P. Yampolskii², M.V. Bermeshev², and N.A. Belov²

¹*Semenov Institute of Chemical Physics RAS, Kosygin st.4, 119991 Moscow, Russia*

²*Topchiev Institute of Petrochemical Synthesis RAS, Leninskii Prosp. 29, 119991 Moscow, Russia*

*email: shant@center.chph.ras.ru

Positron annihilation lifetime spectroscopy (PALS) is a recognized method for the studies of nano-porosity (size distributions of nano-pores) in solids. However, to our knowledge, until recently [1], no special attempts were made to estimate the limits of application of this method to the study of elementary free volumes (EFV). The reason is that, in fact, no alternative methods, applied to the same problem, were discussed. Meanwhile, the studies of nano-porosity are extremely important for creation of novel polymer membrane materials and sorbents with the unique permeation (above 10^3 Barrer for O₂), specific surface (about 10^3 m²/g) and selectivity. The materials are used in solving the problems of ecology, chemistry and medicine. One of contemporary methods, which can be, in some extent, an alternative to PALS, is the low temperature gas sorption (LTGS). In this report, we discuss results of several investigations of polymer membrane materials and sorbents, where the both PALS and LTGS methods are used. Our conclusions on the ranges of application of the two methods are summarised in Table 1 according to pore size (micro-pore or nano-pore) and condition of the material (ready made membrane or powder).

Table 1. Adequacy of PALS and LTGS methods for the studies of porous polymer materials

State of material \ Pore size	Micro-pore <2 nm	Meso-pore 2-50 nm
	(1)	(3)
Powder	PALS, LTGS (<i>HK</i>)	LTGS (<i>BJH</i>)
Membrane	PALS (2)	LTGS (4) (<i>BJH</i>), Sc-CO ₂

HK and *BJH* in brackets indicate Horwath-Kawazoe and Barrett-Joyner-Halenda methods used to analyze low-temperature gas (N₂) sorption (LTGS) curves. Inscription Sc-CO₂ for membrane meso-pore (4) means sorption experiments on creation of meso-porosity in polymers swelled by CO₂ in super-critical (Sc) state. Application of the two methods for EFV studies are determined by different conditions. For example, for PALS, the crucial point is concentration of the trapping centers (10^{18} - 10^{20} g⁻¹), which has to be enough to localize Ps atom before annihilation. For LTGS, materials have to be only in the powder state.

Thus, both methods supplement each other in the research.

[1] V.P. Shantarovich, V.G. Bekeshev, N.A. Belov, *et.al.* High Energy Chem. 50, 300 (2016).

External probing characterization in relation to relaxation dynamics: *cis-1,4-poly(isoprene)*

H. Švajdlénková^{1,*}, O. Šauša², K. Čechová² and J. Bartoš¹

¹Polymer Institute of SAS, Dúbravská cesta 9, 845 41 Bratislava 45, Slovak Republic

²Institute of Physics of SAS, Dúbravská cesta 9, 845 11 Bratislava 45, Slovak Republic

*email: Helena.Svajdlenkova@savba.sk

The structural-dynamic state of amorphous systems can be characterized directly by internal probe techniques such as diffraction, scattering and relaxation, e.g., dielectric spectroscopy. In the indirect characterization, external atomistic (*o*-Ps) and molecular probes may be applied by means of positron annihilation lifetime spectroscopy (PALS) or electron spin resonance (ESR), respectively. Our recent combined PALS and ESR studies on a series of organics with various intermolecular interactions (VdW- vs. H-bonding) [1] and on three *cis-1,4-poly(isoprenes)* (*1,4-PIP*) of different molecular weight [2] revealed the mutual coincidences that suggest the common origin behind the crossover effects in the corresponding PALS and ESR responses.

In our contribution we relate the annihilation behaviour of ortho-positronium (*o*-Ps) in *1,4-PIP 10k* to the spin probe reorientation of 2,2,6,6-tetramethyl-piperidinyl-1-oxyl (*TEMPO*) in *1,4-PIP 10k* via PALS and ESR as well as to the electric dipole relaxation dynamics of the pure medium from broadband dielectric spectroscopy (BDS). The *o*-Ps lifetime over a wide temperature range from 100 K up to 350 K exhibits four regions of different free volume behaviour with three characteristic PALS temperatures: T_g^{PALS} , T_{b1}^L and T_{b2}^L . These findings are in good coincidence with the characteristic ESR bend effects at T_{x1}^{slow} , T_{x2}^{slow} , T_{50G} and T_{x1}^{fast} , T_{x2}^{fast} . Next, relaxation dynamics of *1,4-PIP 10k* as investigated by BDS [3] revealed that the various aspects of the structural relaxation above T_g are responsible for the PALS and ESR crossover effects. Finally, the α -relaxation can be described in terms of the two order parameter (TOP) model [4] with the mutual relationships between $T_m^c \cong T_{b1}^L \cong T_{x1}^{fast}$ and $T_A \cong T_{b2}^L \approx T_{x2}^{fast}$ indicating the common physical origin of the structural-dynamic changes.

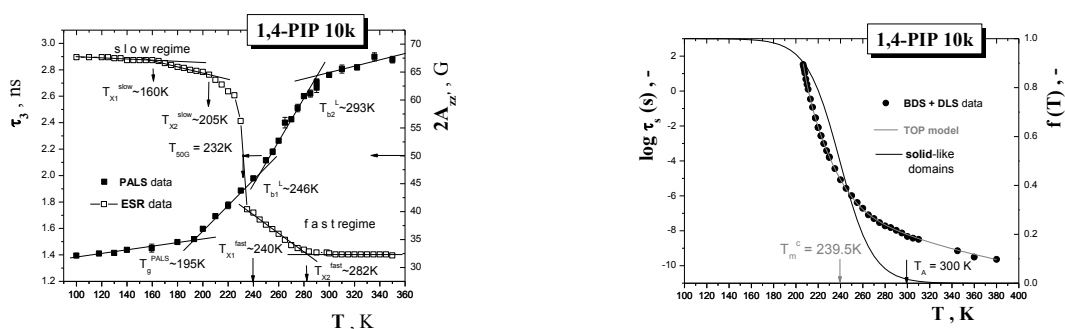


Fig.1. a) Mean *o*-Ps lifetime (τ_3) vs. spectral parameter of *TEMPO* mobility ($2A_{ZZ}$) *1,4-PIP 10k* as a function of temperature b) Structural relaxation time (τ_α) in terms of the TOP model with its characteristics: T_m^c and T_A .

[1] H.Švajdlénková, M.Iskrová-Miklošovičová, V.Majerník, J.Krištiak, J.Bartoš *Chem.Phys.Lett.* 539, 39 (2012)

[2] J.Bartoš, H.Švajdlénková, M.Lukešová, Y.Yu, R.Krause-Rehberg *Chem.Phys.Lett.* 602, 28 (2014)

[3] A. Sokolov, Y.Hayashi, *J.Non - Cryst.Solids* 353, 3838 (2007)

[4] H.Tanaka, *J.Non - Cryst.Solids* 351, 3371, 3385, 3396 (2005)

P13 | Free volume characteristics and thermal properties of thin layers of poly vinyl acetate (PVAc) adsorbed on fumed SilicaS. K. Sharma¹, K. Sudarshan¹, M.Sahu² and P. K. Pujari¹¹Radiochemistry Division, ²Radioanalytical Chemistry Division, Bhabha Atomic Research Centre, Trombay, Mumbai – 400085, India

email: pujari@barc.gov.in

Bulk physical properties like thermal, mechanical and electrical of polymer nanocomposites are shown to be improved as compared to pure polymers [1]. The enhancement in the properties is attributed to the formation of an interfacial layer having distinct molecular packing around the nano-fillers due to interfacial interactions [2]. Characterization of molecular packing of thin polymer layer around nanofillers (interfacial layer) and its role in bulk physical properties of the polymer nanocomposites is an active area of research. In the recent years, it has been shown that positron annihilation lifetime spectroscopy (PALS) can be used to investigate the free volume structure of polymer nanocomposite films. However, it is difficult to obtain the exclusive information about the free volume structure of interfacial layer in the presence of significant amount of bulk like polymer layer [3-6]. In order to investigate the free volume structure of interfacial layer, equivalent thin layers of variable thickness of Poly vinyl acetate (PVAc) have been adsorbed on fumed silica particles from a dilute PVAc solution. A large fraction of positrons implanted in the silica particles diffuse out to their surface where they annihilate within the adsorbed polymer layers. PALS measurements of the PVAc coated fumed silica samples have shown significant changes in the free volume characteristics of the adsorbed layer depending on the amount or thickness of PVAc. Differential scanning calorimetry (DSC) measurements showed the changes in the glass transition process such as shifting in glass transition temperature (T_g) as well as occurrence of two T_g . Thermal gravimetric analysis (TGA) of the coated samples has shown an enhancement in the decomposition temperature of the adsorbed PVAc layers. The observed changes in the thermal properties will be discussed vis- a- vis free volume characteristics of the thin layers.

- [1] A. C Balazs, T. Emrick and T. P. Russell *Science* 314 1107 (2006).
- [2] L. Z. Guan, Y. J. Wan, L. X. Gong, D. Yan, L. C. Tang, L. B. Wu, J. X. Jiang and G. Q. Lai *J. Mater. Chem. A* 2, 15058 (2014).
- [3] S. K. Sharma, J. Prakash, J. Bahadur, K. Sudarshan, P. Maheshwari, S. Mazumder and P. K. Pujari *Phys. Chem. Chem. Phys.* 16, 1399 (2014).
- [4] S. K. Sharma, J. Prakash, K. Sudarshan, D. Sen, S. Mazumder, P. K. Pujari. *Macromolecules* 48, 5706 (2015).
- [5] S. K. Sharma, J. Prakash and P. K. Pujari. *Phys. Chem. Chem. Phys.* 17, 29201 (2015).
- [6] S. K. Sharma, K. Sudarshan and P. K. Pujari. *Phys. Chem. Chem. Phys.* 18, 25434 (2016)

Phase transition behaviour of water confined in titania mesoporesT. Muthulakshmi, D. Dutta, Priya Maheshwari and P. K. Pujari**Radiochemistry Division, Bhabha Atomic Research centre, Mumbai, INDIA*

*email: pujari@barc.gov.in

Phase transition of water under nano-confinement is an active area of research due to its relevance in fundamental physics as well as in biological and technological applications. In the present work, the phase transition behaviour of water confined in titania mesopores with different levels of hydration has been investigated using temperature dependent positron annihilation Doppler broadening and lifetime spectroscopy. The mesoporous titania was synthesized by one-pot sol-gel method using Pluronic F127 as template. The synthesized titania has a pure anatase phase with pore size of 4.8 nm and the BET surface area of 109 m²/g. The titania matrix doesn't favour positronium (Ps) formation. The observed *ortho*-positronium (*o*-Ps) *pick-off* lifetime in hydrated titania represents Ps formation and annihilation in confined water. The change in slope with temperature in the Doppler broadened *S*-parameter and *o*-Ps pick-off lifetime (τ_p) profile is indicative of the phase transition of confined water. It is manifested from the profiles that the phase transition behavior varies with the levels of hydration in titania mesopores. As the hydration level decreases, the H-bonding network among water molecules gets disrupted and the interaction with the pore surface is modified which result in the variation in phase transition behavior. In the fully hydrated titania, water is present both at the surface and the core of the pore, whereas in the partially hydrated pore, the bulk-like core water becomes less. Hence, the effect of surface interaction becomes more prominent as the hydration level decreases. With the decrease in temperature both the τ_p and *S*-parameter values show decreasing trend that saturate at very low temperature limit. In the fully hydrated titania a sharp change in the slope of τ_p is observed just below the bulk freezing point of water (273K) indicative of freezing of bulk like water present in the matrix. A further change in the slope was observed below 250K indicating the ice-nucleation of confined supercooled water. The value of τ_p and the *S*-parameter remain constant below 200K suggesting the completion of the growth of ice nuclei inside the pore. In the partially hydrated titania, on the other hand, the low temperature transition is observed to be extended till 180K. Below 180K, both the τ_p and the *S*-parameter values remain almost constant. The role of hydrogen bonding network on the low temperature phase transition of confined water will be discussed in more details.

P15 | **The combined free-volume and thermal response study of the low hydrated Ca-Montmorillonite**

K. Čechová^{1,*}, O. Šauša¹, I. Matko¹ and K. Jesenák²

¹*Institute of Physics, Slovak Academy of Sciences, Dúbravská cesta 9, 845 11 Bratislava, Slovakia*

²*Faculty of Natural Sciences, Comenius University, Department of Inorganic Chemistry, Mlynská dolina CH-2, 842 15 Bratislava, Slovakia*

*email: katarina.cechova@savba.sk

The common clay mineral, montmorillonite (MMT), belongs to the smectite group of the phyllosilicate minerals. Characteristic features of its structure are high swelling ability because of water absorption. It is used in different areas, e.g. as catalytic processes agent, desiccant to remove moisture, inorganic filler in the polymer industry, etc.

The aim of this study is to characterize free-volume structure in Ca-modified montmorillonite [1,2] at the presence of different amount of water inside of interlayer structure combined with thermoanalytical methods. Free-volume was studied at the samples prepared at simple ambient conditions (room temperature, presence of air). Amount of water was determined by weigh measurements. During the measurements the sample was hermetically sealed. Water desorption process occurring typically between 50°C and 180°C is analyzed in details by thermogravimetric analysis (Perkin Elmer 7). Thermal response of absorbed water for selected steps of desorption process is studied by Differential scanning calorimetry (Perkin Elmer 8500). The correlation of results of characterization methods are provided.

[1] V. Š. Fajnor and K. Jesenák, *J. of Thermal Analysis* 46, 489 (1996)

[2] K. Jesenák, E. Kuchta, L. Guller and J. Fúsková, *Mineralia Slovaca* 29, 439 (1997)

P16 | Controlled porosity of MCM-41 obtained by partial blocking of pores by silicon oil

Marek Gorgol^{1,*}, Jacek Goworek², Patrycja Krasucka², Radosław Zaleski¹,

¹ *Maria Curie-Skłodowska University, Institute of Physics, Department of Nuclear Methods,
Pl. M. Curie-Skłodowskiej 1, 20-031 Lublin, Poland*

² *Maria Curie-Skłodowska University, Faculty of Chemistry, Department of Adsorption,
Pl. M. Curie-Skłodowskiej 3, 20-031 Lublin, Poland*

*email: marek.gorgol@poczta.umcs.lublin.pl

Partial blocking of mesopores in the ordered MCM-41 silica by DC550 silicon oil was proposed as a preparation method of the material with controlled porosity and fixed pore size. The porosity of the samples with various content of DC550 was examined with the use of low temperature nitrogen sorption and positron annihilation lifetime spectroscopy (PALS). It was shown that the oil is good wetting agent for MCM-41 silica. It blocks the primary pores by forming the plugs near its entrances, but also partially locates in the interparticle spaces, especially when primary pores are almost completely filled.

The comparison of the results obtained from both investigation techniques was used to make the first attempt to obtain the calibration (Fig.1) of ortho-positronium intensity, depending on pore volume. This is necessary to improve the utility of PALS as a porosimetric technique. The need to take the migration of positronium to larger free volume into account is discussed. Two proposed curves refer to the situation, when all primary pores are either open (solid line) or closed (dashed line). In most probable case, a fraction of pores is closed, but other fraction remains open, which refers to the area between these curves. One should be noticed, that the calibration could depend on the pore diameter and particular settings of PALS spectrometer. This requires further examination.

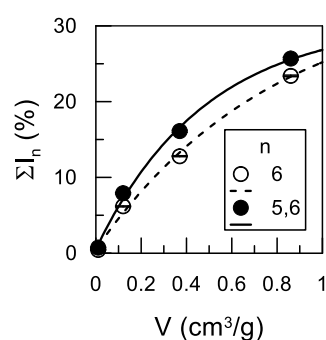


Fig.1 The relation between intensity (I_n) of the components originating from pores of MCM-41 and the total pore volume from nitrogen adsorption.

Positron spectroscopy of nanodiamonds after hydrogen treatment

L.V. Nikitina, R.S. Laptev, A.M. Lider, A.A. Mikhaylov

¹*General Physics Department, Institute of Physics and Technology, Tomsk Polytechnic University, 634000 Tomsk, Russia*

e-mail: gulidova@tpu.ru

The carbon-based material was formed by detonation synthesis (FRPC “Altai”, Byisk, Russia). Synthesis of nanodiamonds is carried out by detonation of solid explosives in an inert atmosphere. The purified material consists of carbon nanodiamonds and onion-like particles. Nanodiamond consists of a crystalline diamond core and nondiamond shell with functional groups on surface.

Hydrogen concentration was measured by Gas Reaction Controller complex (Advanced Materials Corporation, USA) at low temperature and a pressure of 0.6 MPa. The concentration-time sorption isotherms show the concentration of hydrogen absorbed by nanodiamonds.

Investigation of positron lifetime (PL) and Doppler broadening (DB) shift of annihilation line before and after hydrogenation was performed using the special complex. The samples were arranged in a so-called «sandwich» and mounted in a special sample-holder. PL and DB spectra were collected simultaneously. The positron source was represented by a ⁴⁴Ti isotope with an activity of 24.5 μ Ci.

Spectra were fitted using LT10 software. The spectral analysis was performed implementing a delayed formation of positronium (DFP) model. DB spectra were acquired by collecting 2.5×10^5 counts and analyzed using SP software package.

Table 1. The parameters of positron annihilation in the nanodiamonds before and after hydrogenation

Sample	τ_{o-Ps} [ns]	I_{o-Ps} [%]	τ_T [ns]	I_T [%]	τ_{free} [ns]
Initial ND	3.05±0.04	3.35	0.51±0.01	14.8	0.30±0.03
Hydrogenated ND	2.35±0.04	5.07	0.42±0.01	42.3	0.29±0.02

The nanodiamonds hydrogen saturation leads to change the lifetime of trapped positrons and ortho-positronium, intensity, S and W-parameters.

Consequently, these results show that positron spectroscopy can be used to study carbon hydrogen storage materials.

Positronium probing of pores in zirconia nanopowders

I. Prochazka^{1,*}, J. Cizek¹, F. Lukac¹, O. Melikhova¹, P. Hruska¹, W. Anwand², O. Liedke², T.E. Konstantinova³ and I.A. Danilenko³

¹*Department of Low Temperature Physics, Faculty of Mathematics and Physics, Charles University, V Holesovickach 2, CZ-180 00 Praha 8, Czech Republic*

²*Institute of Radiation Physics, Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstr. 400, 01328 Dresden, Germany*

³*National Academy of Sciences of Ukraine, Donetsk Institute for Physics and Engineering Named after O. O. Galkin, Luxemburg Street 72, 83114 Donetsk, Ukraine*

*email: ivan.prochazka@mff.cuni.cz

Zirconium di-oxide (ZrO_2 , zirconia) receives nowadays a big attention because of a variety of advantageous properties which make zirconia-based materials useful in numerous fields of practice, in particular, in ceramic industry and other high-temperature applications. To make high-temperature phases of zirconia stabilised down to room temperature, doping of the host lattice by proper metal cations has to be usually performed. Nanopowders are currently focused on as starting substances for manufacturing ZrO_2 -based ceramics by sintering, because well-homogenised materials of a low porosity can be produced more easily. Nanometer-sized defects associated to grain boundaries (GBs) become then to play an enhanced role in nanopowders due to enlarged volume fraction of GBs. Positrons and positronium (Ps) atoms can serve as efficient probes of different structures encountered in particular stages of manufacturing ZrO_2 -based functional materials.

In the present contribution, conventional positron and Ps lifetime measurements were carried out on a variety of zirconia-based nanopowders and ceramics obtained by sintering these nanopowders. Nanopowders studied were doped with various metal cations (Y^{3+} , Cr^{3+} , Ce^{4+} , Mg^{2+}) and differed also in thermal treatment prior sintering. Lifetime experiments were conducted in air or in vacuum and combined with Doppler broadening measurements using slow-positron beam and supplemented with X-ray diffraction (XRD) and mass-density (MD) measurements. In Figure, variability of the lifetime spectra observed is illustrated. In a range of lifetimes from a few ns to ≈ 70 ns, up to three individual lifetime components could be identified, see Figure, (a) and (b). Such observations unambiguously testified Ps formation with subsequent ortho-Ps annihilation. On the other hand, an absence of the ortho-Ps components was found in certain nanopowders giving thus an evidence of a strong Ps inhibition, see Figure, (c).

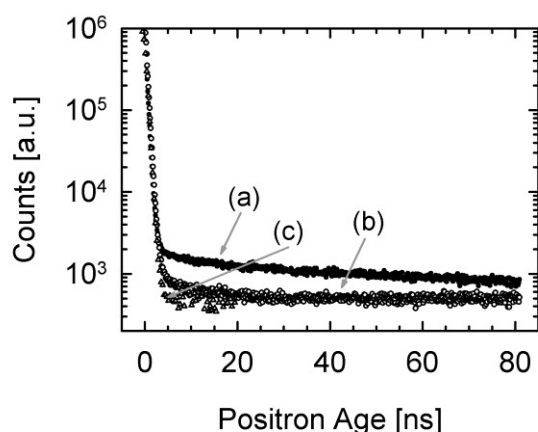


Figure. Lifetime spectra measured in air for ZrO_2 nanopowders doped with (a) 10 mol.% MgO , (b) 12 mol.% CeO_2 and (c) 3 mol.% Cr_2O_3 .

Pore sizes were estimated using current models of correlation between observed ortho-Ps lifetime and pore size. Origins of pores will be discussed on the basis of the ortho-Ps data in combination with the results of slow-positron beam, XRD and MD measurements.

P19 | Pores in various kinds of zeolites by positron annihilation spectroscopy

 N. Sakata^{1*}, A. Nozaki¹, L. Chiari¹, M. Fujinami¹
¹Department of Applied Chemistry, Chiba University, 1-33 Yayoi, Inage, Chiba, Japan

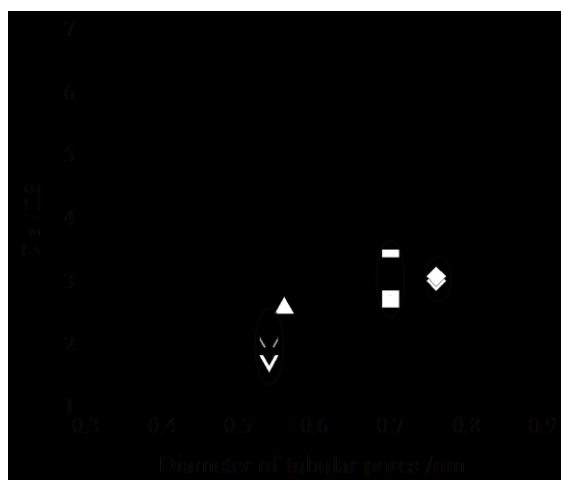
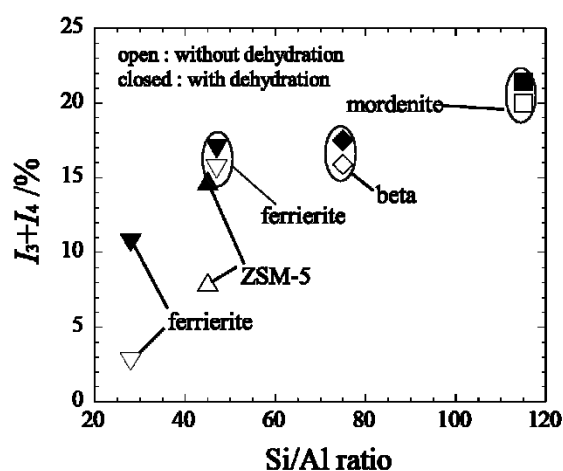
*email: nagisa.sakata@chiba-u.jp

Zeolite is a porous material with regular tubular pores (0.4-0.8 nm diameter) and cavities with the basic unit of tetrahedral (SiO₄)⁴⁻ and (AlO₄)⁵⁻. There are various crystal structures, and it is known that chemical properties such as catalytic activity and ion exchange species change with different Si/Al ratios and crystal structures. In this study, we have measured the Ps behavior, such as lifetime and formation rate, and correlated them with the crystal structure and the Si/Al ratio.

Positron annihilation lifetime spectroscopy (PALS) was carried out on ZSM-5 and ferrierite, both having a 10-membered ring, as well as beta and mordenite, both of which possess a 12-membered ring. Zeolite powder was molded into pellets having a diameter of 10 mm and a thickness of 2 mm. Subsequently, all samples underwent vacuum heating at 458 K for 2 hours in order to dehydrate them. Finally, a dehydrating agent and an oxygen scavenger were enclosed in a thermally sealed polyethylene bag together with each sample and the positron lifetimes were measured under these controlled atmosphere conditions. Each measured spectrum was fitted using four lifetime components. The 3rd component (of the order of ns) and 4th component (of the order of tens of ns) are due to the annihilation of o-Ps.

The PALS results for the zeolites except ZSM-5 showed that the pick-off lifetime of o-Ps without dehydration was well correlated with the diameter of the tubular pores (Fig. 1). On the other hand, the dehydration process led to a longer o-Ps lifetime. The adsorbed water in the tubular pores hindered the diffusion of Ps, so that the o-Ps lifetime actually reflected the diameter of the pores with adsorbed water. We concluded that Ps can more easily diffuse in the cavities by dehydration and thus the o-Ps lifetime becomes longer.

An increase in Al³⁺ ions gives rise to an addition of polar groups in the tubular pores. The plot of the sum of I₃ and I₄ vs Si/Al ratio is shown in Fig. 2. The higher the Si/Al ratio, the larger is the Ps formation component. Furthermore, the dehydration led to an increase of the Ps formation intensity. This result was expected given that electrons and positrons tend to be captured by the adsorbed water, leading to a decrease of the Ps formation probability.


 Fig. 1 Plot of τ_3 vs diameter of tubular pores.

 Fig. 2 Plot of I_3+I_4 vs Si/Al ratio.

Porosity of silica monoliths with tailored mesopores of ink bottle shape determined by nitrogen adsorption and positron annihilation lifetime spectroscopy

Andrzej Sienkiewicz¹, Agnieszka Kierys¹, Marek Gorgol², Radosław Zaleski^{2,*}

¹ *Maria Curie-Skłodowska University, Faculty of Chemistry, Department of Adsorption, Pl. M. Curie-Skłodowskiej 3, 20-031 Lublin, Poland*

² *Maria Curie-Skłodowska University, Institute of Physics, Department of Nuclear Methods, Pl. M. Curie-Skłodowskiej 1, 20-031 Lublin, Poland*

*email: radek@zaleski.umcs.pl

The comparison of pore size distributions obtained with the use of two porosimetric methods: low temperature nitrogen sorption (LN2) and positron annihilation lifetime spectroscopy (PALS), was performed for porous silica monoliths. Four investigated samples were prepared under various synthesis conditions. Nitrogen sorption showed the presence of bottle-shaped pores in all investigated samples. In addition, it seems, that the presence of methanol during synthesis influences porosity to a greater extent than organic additives.

Quite good agreement between the LN2 and PALS results was observed only for the silica monolith synthesized with β -cyclodextrins as pore directing agent. The biggest discrepancy in the results obtained from these two techniques was observed for the silica gel synthesized with no additives. The origin of such discrepancies, taking into account the shape of pore size distribution and deficiencies of data analysis techniques, is discussed.

P21 | **A two-particle model for Positronium confined in sub-nanometric cavities**

G.M.Tanzi^{1,*}, F.Castelli^{1,2} and G.Consolati^{2,3}

¹*Department of Physics, Università degli Studi di Milano, via Celoria 16, I-20133 Milano, Italy*

²*INFN, sezione di Milano, via Celoria 16, I-20133 Milano, Italy*

³*Department of Aerospace Science and Technology, Politecnico di Milano, via LaMasa 34, I-20156 Milano, Italy*

*email: giacomo.tanzi@unimi.it

In the last years, the electron-positron bound state, namely the positronium atom (Ps), has been widely used as a probe to test structural properties of porous materials. This is possible thanks to the strong connection between Ps annihilation rate and the electronic structure of the confining medium.

Accessible experimental measurements concern annihilation rates by pickoff processes and contact densities (the electron density at the positron position).

While the pickoff process is well understood, existing models describing Ps properties in nanometric or sub-nanometric cavities fail to justify the lowering of the contact density with respect to that of Ps in vacuum, as found in most materials.

For this reason we formulated a new two-particle model in which only the electron is confined in the cavity [1], while the positron is moving freely and feels the medium via a positive work function. We show that this model explains experimental data for a large class of materials and suggests a way to gain information on pore sizes and positron work functions.

[1] G. Marlotti Tanzi, F. Castelli, and G. Consolati, *Phys. Rev. Lett.* 116, 033401 (2016)

Evaluation of e^+ implantation profile for ^{22}Na positron source

Akmalova Yu.A.¹, Dubov L.Yu.^{1,2}, Stepanov S.V.^{1,2}, Yu.V. Funtikov², Shtotsky Yu.V.^{1,2}

¹ National Research Nuclear University "MEPhI", Moscow, Russia

² NRC "Kurchatov Institute" Institute of Theoretical and Experimental Physics, Russia

*email: YAAkmalova@mephi.ru

To employ positrons emitted from isotope sources for analysis of near-surface layers of solid-state materials one needs to account for their range, which usually varies from tens to hundreds of microns. Therefore using isotope sources for positron annihilation lifetime spectroscopy (PALS) requires accurate information on positron implantation profiles (PIPs). Usually PIPs are described as monoexponential distributions, however in some publications [1] the authors note that these profiles have more complex shape.

In current work we present the results of Geant4 simulation of PIPs for materials with different densities (Fig. 1). We simulate a standard geometry for PALS measurements: the positron source is placed between two 1 mm thick samples. The source represents a radioactive NaCl layer of 1 μm thickness covered by a 8 μm kapton films.

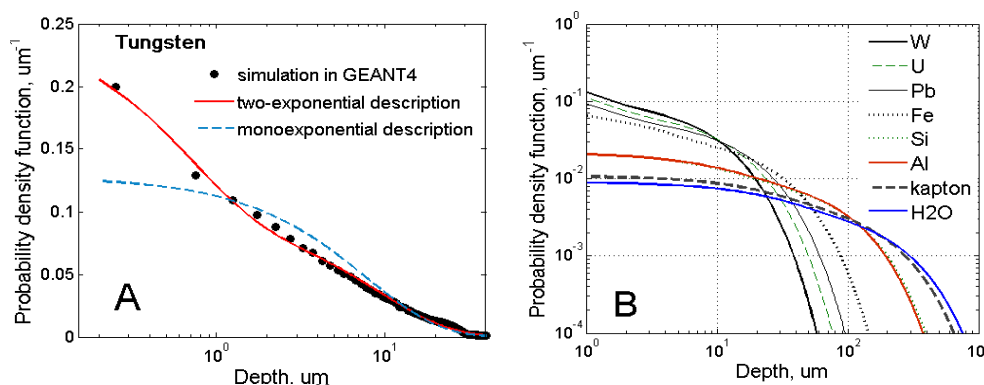


Fig.1. Implantation profiles for ^{22}Na source: A) comparison of conventional and two-exponential description for tungsten; B) materials with different densities.

The shape of PIP depends on both energy and angular distributions of the positrons entering the sample. The results of simulation show that the positron probability density function can be described by the sum of two exponential components (Fig. 1a). The fraction of a short-depth component for all studied materials is found to be around 11% and thus implantation profiles can be expressed as follows:

$$f(x) = 0.11 \cdot a \cdot e^{-ax} + 0.89 \cdot b \cdot e^{-bx}, \quad (1)$$

where x [μm] is the depth of the sample and prefactors a and b [μm^{-1}] can be approximated as functions of the studied materials density ρ [g/cm^3] as:

$$a = 0.0024 \cdot (\rho - 0.3)^2 + 0.045 \cdot (\rho - 0.3), \quad b = 0.0056 \cdot (\rho - 0.2), \quad (2)$$

Finally, we verify our Geant4 simulations experimentally by measuring the fraction of the positrons passed through the thin films using PALS technique and confirm the proposed model of PIP.

[1] J. Dryzek and K. Siemek J. Appl. Phys. 114, (2013)

P23 | Simulations on reducing the influence of backscattered slow positrons on lifetime measurements.

D. Dinescu^{1,2*}, and N. Djourellov¹

¹ *Extreme Light Infrastructure - Nuclear Physics, Horia Hulubei National Institute for Physics and Nuclear Engineering, 30 Reactorului Street, 077125 Magurele, Ilfov county, Romania*

² *University Politehnica of Bucharest, Applied Science College, Splaiul Independentei, nr. 313, 060042, Bucuresti, Romania*

*email: Doru.Dinescu@eli-np.ro

For the development of new functional materials, the investigation of lattice defects and various atomic imperfections in solids constitutes an important step. For analyzing subsurface layers and thin films, slow e^+ beams are necessary. At the European Light Infrastructure – Nuclear Physics (ELI-NP), a brilliant γ -beam will produce fast e^+ by the pair production in a suitable converter made of tungsten foils, which will also act as a moderator [1]. One of the positron annihilation techniques, which over the years has become an increasingly valuable tool for study of the defect structure in materials is the Positron Annihilation Lifetime Spectroscopy (PALS). In order to perform PALS with a slow e^+ beam a start signal is needed. For obtaining the start signal, at ELI-NP, the slow e^+ beam will be pulsed using the chopping and bunching technique [2]. For depth profiling purposes, the slow e^+ are accelerated by a few graded electrodes to a desirable energy up to typically 30 keV.

When incident e^+ hit the target a fraction of them is backscattered. If the backscattered e^+ reach back the accelerator they can be reflected by the electric field and implanted into the sample with a delay from the initial e^+ bunch. Despite their small overall contribution, the caused satellite structures can make the spectrum analysis difficult.

The method implemented at the EPOS beam line of guiding the e^+ through a 45° bent tube equipped with steering coils after they pass the accelerator will not allow the e^+ backscattered from the target to reach the acceleration field [3]. The same method will be implemented at the ELI-NP e^+ line. To understand the origin of these satellite structures and to further improve the performance of the system, comprehensive simulations were performed in Comsol Multiphysics and Geant4. The aim of the study conducted in the present paper is to determine the optimum parameters of the designed system in order to obtain PALS spectra with minimum distortions caused by the backscattered e^+ .

[1] N. Djourellov, C. Hugenschmidt, S. Balascuta, V. Leca, A. Oprisa, C. Piochacz, C. Teodorescu and C. A. Ur, *Romanian Reports in Physics* 68, S735 (2016)

[2] N. Djourellov and D. Dinescu, *J. Phys.: Conf. Series* 791, 012010 (2017)

[3] M. Jungmann, J. Haeberle, R. Krause-Rehberg, W. Anwand, M. Butterling, A. Wagner, J. M. Johnson and T. E. Cowan, *J. Phys.: Conf. Series* 443, 012088 (2013)

Positronium lifetime measurement using J-PET Detector

Kamil Dulski^{1*} on the behalf of J-PET collaboration

¹*Nuclear Physics Institute, Jagiellonian University, Lojasiewicza 11, 30-348 Cracow*

*email: kamil.dulski@gmail.com

Positron Annihilation Lifetime Spectroscopy (PALS) is a great tool to study nanostructure of porous materials. Iterative computer procedure based on LT and MELT was prepared to analyze positron lifetime spectra and to extract average positronium lifetimes distribution. Specific iteration method which is based on increasing number of components fitted to spectrum in each step helped stabilize and accelerate operation of fitting program. Procedure uses ROOT software and Levenberg-Marquadt algorithm to retrieve mean lifetime distribution with additional information about dispersion of main components. Two exemplary samples, silicon plates (Si) and polyvinyl toluene (PVT) were measured in order to check analysis procedure. Nanostructural information received from PALS analysis putted into the metabolic image obtained by Positron Emission Tomography (PET) can give a quite new quality of imaging of the human body. Proposition of joining PET and PALS techniques altogether in J-PET device is briefly described.

A. Gajos, E. Czerwiński, D. Kamińska, P. Moskal, Patent: PCT/PL2015/050038

P. Moskal et al., Acta Phys.Polon. B47 (2016) 509

B. Jasińska et al., Acta Phys.Polon. B47 (2016) 453

A. Gajos et al., Nucl. Instrum. Meth. A819 (2016) 54.

D. Kamińska et al., Nukleonika 60 (2015) 729.

P. Moskal et al., Nucl. Instrum. Meth. A775 (2015) 54.

P. Moskal et al., Nucl. Instrum. Meth. A764 (2014) 317.

P25 | **Reconstruction of hit-time and hit-position of annihilation quanta in J-PET detector using synchronized model signals**

N. G. Sharma^{1*} for J-PET collaboration

¹ *Faculty of Physics, Astronomy and Applied Computer Science, Jagiellonian University, 30-348 Cracow, Poland*

* email: pnp.neha@gmail.com

The Jagiellonian Positron Emission Tomograph is an cost-effective scanner [1] being developed at the Jagiellonian University, Krakow. It is composed of long strips of organic scintillators. This detecting system is also capable to study the decays of positronium atoms [2]. In the J-PET detector the amplitude of signals used for reconstruction is strongly dependent on the hit-position of gamma quanta, not on the energy deposited by it. Therefore, a novel reconstruction method based on the comparison of examined signal with the model signals stored in the library using Mahalanobis distance has developed [3]. The method has validated on two strip J-PET module. In the present article results obtained from the validation of reconstruction method will be presented and discussed.

Keywords: J-PET detector, J-PET two strip module, mahalanobis metric

[1] P. Moskal, Patent granted in 2014, Nos. EP2454612B1, WO2011008119, EP2454611, WO2011008118.

[2] P. Moskal et al., Acta Phys. Polon.B 47 509 (2016).

[3] N. G. Sharma et al., Nukleonika, 60 765 (2015).

P26 | Surface Studies at SPF, KEK: Positron Diffraction and Positronium TOF

T. Hyodo^{1,*}, I. Mochizuki¹, A. Ichimiya¹, M. Kimura¹, N. Toge², T. Shidara², Y. Fukaya³,
S. Shamoto³, K. Wada⁴, M. Maekawa⁴, A. Kawasuso⁴, M. Fujinami⁵, T. Shirasawa⁶,
T. Takahashi⁷, H. Ariga⁸, K. Asakura⁸, S. Iida⁹ and Y. Nagashima⁹

¹*Institute of Materials Structure Science, KEK, Tsukuba, 305-0801, Japan*

²*Accelerator Laboratory, KEK, Tsukuba, 305-0801, Japan*

³*Advanced Science Research Center, JAEA, Tokai, 319-1195, Japan*

⁴*Quantum Beam Science Center, QST, Takasaki, 370-1292, Japan*

⁵*Department of Applied Chemistry, Chiba University, Chiba, 263-8522, Japan*

⁶*Research Institute for Material and Chemical Measurement, AIST, Tsukuba, 305-8569, Japan*

⁷*Tokyo Gakugei University, Koganei, 184-8501, Japan*

⁸*Institute of Catalysis, Hokkaido University, Sapporo, 305-8569, Japan*

⁹*Department of Physics, Tokyo University of Science, Tokyo 162-8601, Japan*

* email: hyodot@post.kek.jp

Recent Surface studies at the Positron Facility (SPF) in IMSS, KEK are reported. The slow-positron beams of intensity $5 \times 10^7/\text{s}$ in the long-pulse mode (width 1.2 μs) and $5 \times 10^6/\text{s}$ in the short-pulse mode (1-10 ns, variable) are stably used.

1. Positron diffraction: Total-reflection high-energy positron diffraction (THREPD) is a unique method exceedingly sensitive to the atomic geometry of the topmost- and immediate sub-surface [1,2]. Recent results using the long-pulse mode positron beam are the determination of the graphene-substrate distance where the substrates are Cu(111) and Co(0001)[3], and the detection of an asymmetric buckling structure of germanene on Al(111)[4]. It also determined a surface atomic structure of rutile-TiO₂ (110)(1×2), which had been debated for more than 30 years [5].

A low-energy positron diffraction (LEPD) station using the long-pulse mode positron beam has been constructed and a diffraction pattern from Ge(001)(2×1) surface was observed. The pattern is recorded by a delay-line detector (DLD). Since a DLD does not accept too many positrons in a short pulse, a technique has been developed to stretch the 1 μs pulse to an appropriate width up to 20ms.

2. Positronium time-of-flight (Ps-TOF): Ps-TOF station is operated with the beam in the short pulse mode whose width is short enough for the measurement of TOF of the ortho-Ps whose lifetime is 142 μs . For metals, in particular, the spectrum carries information on the electronic state of the surface exclusively, because Ps does not form in the bulk and thus it is certain that the Ps emitted is formed on the very surface. Recently it was observed that coating of W surface with alkali metals greatly enhanced the Ps emission from the surface [6]. The energy spectra show evidence of energy loss compared to that of the Ps emitted from a clean W surface.

This study was performed under the PF Proposal No.2016S2-006, 2014S2-004, 2013S2-005 and 2013U002, and the auspices of the JAEA-KEK Joint Development Research at KEK. It was partly supported by JSPS grants KAKENHI (S)24221006 and (S)24221007 and those for Young Scientists (B) 25800182 and 26800170, Cabinet office Cross-ministerial Strategic Innovation Promotion Program (SIP, unit D66), and by Toray Science and Technology Grant from Toray Science Foundation.

[1] Y. Fukaya, et al., Appl. Phys. Express 7, 056601 (2014).

[2] C. Hugenschmidt, Surf. Sci. Rep. 71, 547 (2016).

[3] Y. Fukaya, et al., Carbon 103, 1 (2016).

[4] Y. Fukaya, et al., 2D Materials, 3, 035019 (2016).

[5] I. Mochizuki et al., Phys. Chem. Chem. Phys., 18, 7085 (2016).

[6] S. Iida, et al., J. Phys.: Condens. Matter 28, 475002 (2016).

Improvements in the Production of ²²Na Positron Sources at iThemba LABS

C. Naidoo^{1,*}, R. Krause-Rehberg²

¹*iThemba Labs, Old Faure Road 1, Faure 7131, South Africa*

²*Univ. Halle, Inst. of Physics, 06099 Halle, Germany*

*email: clive@tlabs.ac.za

The poster shows the production of ²²Na at the iThemba Labs in Faure (near Cape Town) and the improvements recently obtained.

iThemba LABS has been producing ultra-high vacuum (UHV) ²²Na positron sources since the mid 1990's. Today, iThemba LABS is the only producer of these UHV ²²Na positron sources worldwide. These sources are produced by using the in-house produced high purity ²²Na radionuclide with a specification of >800 Ci ²²Na per gram of sodium together with the empty source capsules produced by Rehberg Electronics (Prof. Dr. Reinhard Krause-Rehberg) in Halle, Germany.

In the last quarter of 2014, we encountered a few problems from clients complaining about the low beta efficiency of the ²²Na positron sources. This paper will present the improvements made by Rehberg Electronics on the empty source capsule together with the improvements made by iThemba LABS on the dispensing of the ²²Na radionuclide during the manufacture of the ²²Na source capsule. Since the implementation of these improvements, the quality of the ²²Na positron sources has improved drastically and we have only received positive feedback from clients in this regard. In addition, upgrades of the current ²²Na production facility, the availability of the ²²Na stock levels together with the future vision of iThemba LABS will also be presented.

The semi-digital spectrometric system for positron spectroscopyR.S. Laptev^{1*}, A.A. Mikhaylov¹, Y.S. Borbulev¹, G.V. Garanin¹ and A.M. Lider¹¹*Department of General Physics, National Research Tomsk Polytechnic University, Tomsk 634050, Russia*

*email: laptevrs@tpu.ru

Positron spectroscopy (PS) methods are the most promising for controlling the defect structure of hydrogen containing systems due to high sensitivity and the ability to determine the type of defects and concentration. However, despite the potential capabilities of PS methods, their use is severely limited due to the low counting rate and the lack of techniques for decoding and interpreting the data, especially for metal-hydrogen systems.

To study the evolution of the defect structure of metals and alloys upon hydrogen saturation, a completely digital spectrometric complex has been developed in which the methods of positron lifetime spectrometry and the coincidence analysis of the Doppler broadening of the annihilation line are integrated [1,2]. The main disadvantage of a fully digital spectrometric channel is the presence of a large number of background events in the spectrum, which significantly increases the size of the received file (up to 3 TB) and increases processing time (several tens of hours).

To eliminate this drawback, external trigger (ET) systems are developed for each module. The external circuit carries out preliminary selection of signals and forms a control pulse, which then arrives at the trigger of the digitizer trigger. Thus, the digitizer performs further processing of only "useful" signals. The disadvantage of such systems is that additional devices (amplifiers, discriminators, coincidence circuit, etc.) that complicate the setup and operation of the spectrometer and also increase its cost are required for preliminary selection. The use of external synchronization systems reduces the rate of signal collection, but increases the efficiency of their processing.

The use of analog devices in the digital spectrometric complex slightly increases the cost of the complex and makes it difficult to configure, but it allows to significantly improve its characteristics. A semi-digital complex of positron spectroscopy with an external synchronization system based on the positron lifetime spectrometry modules and coincidence Doppler broadening spectrometry (CDBS) has the following technical characteristics using a positron source based on the ⁴⁴Ti isotope with the activity of 0.91 MBq:

- the time resolution of the digital lifetime module is 170 ± 7 ps, the counting rate (90 ± 30) s/s
- The energy resolution of the CDBS module is (1.16 ± 0.03) keV, the counting rate (116 ± 15) ss / s.

[1] Bordulev Y. et al. Development of a digital spectrometric system for material studying by positron annihilation techniques //Strategic Technology (IFOST), 2012 7th International Forum on. – IEEE, 2012. – C. 1-4.

[2] Laptev R. S. et al. Gas-phase hydrogenation influence on defect behavior in titanium-based hydrogen-storage material //Progress in Natural Science: Materials International. – 2017. – T. 27. – №. 1. – C. 105-111.

Development of sample holders with thin SiN windows for PALS measurement of liquid samples

Brian E. O'Rourke¹*, Nagayasu Oshima¹, Yuji C. Sasaki²

¹National Metrology Institute of Japan, National Institute of Advanced Industrial Science and Technology (AIST), 1-1-1 Umezono, Tsukuba, Ibaraki 305-8568, Japan

²Department of Advanced Materials Science, Graduate School of Frontier Sciences, The University of Tokyo, 5-1-5 Kashiwanoha, Kashiwashi, Chiba 277-8561, Japan

*email: brian-orourke@aist.go.jp

At AIST we have used thin SiN windows to extract a slow positron beam from the vacuum chamber into atmosphere for in-situ positron annihilation lifetime spectroscopy (PALS) measurement of thin films as a function of humidity [1,2]. In principle this system can also be applied to the measurement of liquids by placing the liquid sample on the outside of the window. However, measurements with the focussed microbeam are time consuming and difficult to set-up. In addition, the window is fragile and a failure would lead to a catastrophic loss of vacuum integrity and possible damage to pumps etc.

In order to mitigate these disadvantages we have started to develop small liquid holders which can be placed into the vacuum chamber in a similar way to a typical sample. The liquid is placed in the centre of the holder and covered with a thin SiN window which is sealed with a rubber o-ring. As this system is designed to be used with an unfocussed positron beam, it is necessary to use somewhat thicker windows (~200 – 500 nm) as compared to those possible with the microbeam (~30 nm). The increased thickness requires a corresponding increase in beam energy in order to ensure most positrons annihilate in the sample rather than the window [3].

With this holder, we plan to perform PALS on a range of liquids. By varying the positron energy it is possible to vary the ratio of positrons which annihilate in the window compared to the liquid and hence observe any change in lifetime in the solid/liquid interface region compared to the bulk liquid. We will report preliminary measurements using these newly developed holders at the meeting.

[1] W. Zhou *et al.*, *Appl. Phys. Lett.* 101, 014102 (2012).

[2] W. Zhou *et al.*, *J. Phys. Conf. Ser.* 443 012090 (2013)

[3] B. E. O'Rourke *et al.*, *J. Phys. Conf. Ser.* 443 012069 (2013)

J-PET detector NEMA spatial resolution studies

M. Pawlik-Niedźwiecka^{1,*}, Sz. Niedźwiecki¹ on behalf of J-PET collaboration

¹*Faculty of Physics, Astronomy and Applied Computer Science, Jagiellonian University,
prof. Stanisława Łojasiewicza 11, 30-348 Kraków*

* email: monika.pawlik@doctoral.uj.edu.pl

J-PET detector, based on long plastic scintillator strips, was recently constructed in Jagiellonian University [1]. It consists of 192 modules axially arranged into three layers, read out from both sides by digital constant-threshold boards. Each signal is probed at four different thresholds. Synchronization detection modules has been completed with a reference detector placed inside scanner.

J-PET scanner may be licensed for commercial use after fulfilling standards defined by The National Electrical Manufacturers Association (NEMA). To determine performance characteristics of J-PET detector a NEMA-NU-2 [2] norms are used which specify the standard values of the spatial resolution, signal-to-background ratio and scattered gamma fraction. Therefore, it is necessary to carry out appropriate testing of the J-PET prototype which results will be used for device certification [3].

In this poster initial results of the J-PET spatial resolution will be presented for ²²Na source placed at selected positions inside the detector chamber as well as time and energy resolutions for detection modules.

[1] P. Moskal, Sz. Niedźwiecki et al., Nuclear Instruments and Methods in Physics Research Section A 764, 317 (2014)

[2] NEMA-NU-2 standard - <https://www.nema.org/>

[3] L. Raczyński et al., Physics in Medicine & Biology 62, 5076 (2017)

P31 | **Optimization of positron-lifetime measurement geometry based on Geant4 simulations**

M. Saro^{1,*}, M. Petriska¹ and V Slugeň¹

*Institute of Nuclear and Physical Engineering, Slovak University of Technology, Ilkovičova 3,
81219 Bratislava, Slovakia*

*email: matus.saro@stuba.sk

Proper choice of measuring geometry and experimental setup of nuclear instrumentation modules and photomultipliers is key element which affects substantial measurement properties: count rate and time resolution. An adequate compromise has to be found, when it comes to geometry of measurement. The optimal geometry using three detector layout is inspected in this paper. During our work, we concentrated on the simulation of XP2020Q photomultipliers and the BaF2 scintillator material. The Geant4 simulation allows to estimate an influence of the measuring geometry on detection efficiency and to choose the most appropriate crystals dimensions and positions. As mentioned in [1], slight changes in geometry result in distortion or improvement of measured results. Experimental results already showed, changes of start crystals dimensions can result in significant increase in count rate of three-detector measurement.

Acknowledgment:

This article was created with the support of VEGA 1/0339/16 and 1/0104/17.

- [1] L.Yu. Dubov, V.I. Grafutin, Yu.V. Funtikov, Yu.V. Shtotsky, L.V. Elnikova, *Optimization of BaF2 positron-lifetime spectrometer geometry based on the Geant4 simulations*, Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, Volume 334, (2014), ISSN 0168-583X

P32 | Time over Threshold (TOT) as a measure of Energy deposition by gamma quanta in plastic scintillator used in J-PET

J. Raj¹, K. Kacprzak¹, Sushil K. Sharma^{1*} for J-PET collaboration

¹ *Faculty of Physics, Astronomy and Applied Computer Science, Jagiellonian University, 30-348 Cracow, Poland*

* email: sushil.sharma@uj.edu.pl

The Jagiellonian Positron Emission Tomograph (J-PET) [1-4] is one of its kind based on the organic scintillators developed at Jagiellonian University in Krakow. The organic scintillators are hydrocarbon compounds, therefore, the gamma quanta interact predominantly via the Compton effect. The energy loss of incident photon in scintillator varies with scattering angle of outgoing photon. In this study, we present a method to establish a relationship between the maximum energy deposited by incoming gamma quanta in plastic scintillator and sum of the Time Over Threshold (TOT) spectra estimated from the signals measured from scintillator by using photomultiplier tubes and associated electronics. Such a study is also of utmost importance to distinguish the origin of photons i.e., either annihilation or de-excitation process.

Keywords: J-PET, Time Over Threshold (TOT), Plastic scintillator.

[1] 18 Patent Applications, <http://koza.if.uj.edu.pl/patents/>.

[2] P. Moskal et al., Nucl. Inst. and Meth. A 764 (2014) 317.

[3] M. Pałka et al., Bio Algorithms and Med-Systems 10 (2014) 41.

[4] G. Korcyl et al., Bio-Algorithms and Med-Systems 10(2014) 37.

P33 | Measurement of gamma quantum interaction point in plastic scintillators with WLS strips

Shivani^{1,*}, J.Smyrski¹, for the J-PET Collaboration¹

¹*Faculty of Physics, Astronomy and Applied Computer Science, Jagiellonian University,
S. Łojasiewicza 11, 30-348 Cracow, Poland*

*email: shivanichdhr6@gmail.com

The feasibility of measuring the axial co-ordinate of a gamma quantum interaction point in a plastic scintillator bar via the detection of scintillations photons escaping from the scintillator with an array of wavelength-shifting (WLS) strips is demonstrated. Using a test setup comprising a BC-420 scintillator bar and an array of 16 BC-482A WLS strips. We achieved a special resolution of 5mm (σ) for annihilation photons from a ²²Na isotope. The studied method can be used to improve the special resolution of a plastic scintillator based PET scanner which is being developed by the J-PET collaboration.

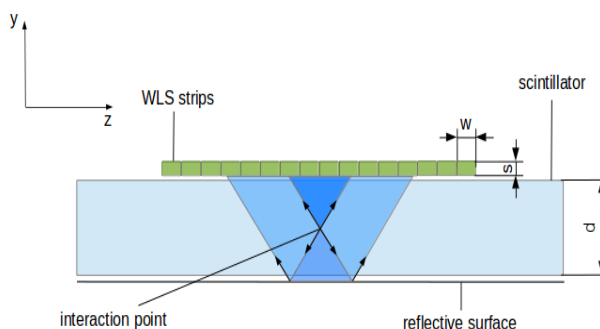


Fig.1. Principle of measuring the axial coordinate of the gamma quantum interaction point in a plastic scintillator bar using an array of WLS strips.

- [1] J. Smyrski, et al. Nucl. Instrum. Methods A 851 (2017) 39-42.
- [2] N.N. Shehad, et al. IEEE 2005 Nuclear Science Symposium Conference Record 5, 2005, pp. 2895-2898.
- [3] S.J. Park, et al. Nucl. Instrum. Methods A 570 (2007) 543-555.
- [4] T.J. Smyrski, et al. Nucl. Instrum. Methods A 851 (2017) 39-42.
- [5] A. Miceli, et al. Phys. Med. Biol. 57 (2012) 1685-1700.
- [6] P. Moskal, et al. Nucl. Instrum. Methods A 764 (2014) 317.
- [7] P. Moskal, et al. Phys. Med. Biol. 61 (2016) 2025-2047.
- [8] J. Smyrski, et al. BioAlgorithms Med. Syst. 10 (2014) 59-63.

J-PET time calibration

M. Skurzok^{1,*} for the J-PET Collaboration

¹*Faculty of Physics, Astronomy and Applied Computer Science, Jagiellonian University,
30-348 Cracow, Poland*

*email: magdalena.skurzok@uj.edu.pl

The Jagiellonian Positron Emission Tomograph (J-PET) project carried out in the Institute of Physics of the Jagiellonian University is focused on construction and tests of the first prototype of PET scanner for medical diagnostic which allows for the 3D imaging of the whole human body using organic scintillators. J-PET prototype consists of 192 scintillator strips forming three cylindrical layers which are optimized for the detection of photons from the electron-positron annihilation with high time- and high angular-resolution.

The poster presents the method of the time calibration and synchronization of the whole detection system based on the measurements performed with a ²²Na radioactive source and a reference detector.

- [1] J-PET: P. Moskal et al., *Acta Phys. Polon. B* 47, 509 (2016)
- [2] J-PET: A. Gajos et al., *Nucl. Instrum. Meth. A* 819, 54 (2016)
- [3] J-PET: D. Kamińska et al., *Eur. Phys. J. C* 76, 445 (2016)
- [4] J-PET: P. Moskal et al., *Phys. Med. Biol.* 61, 2025 (2016)
- [5] J-PET: P. Moskal et al., *Nucl. Instrum. Meth. A* 775, 54 (2015)
- [6] J-PET: P. Moskal et al., *Nucl. Instrum. Meth. A* 764, 317 (2014)
- [7] J-PET: J. Smyrski et al., *Nucl. Instrum. Meth. A* 851, 39 (2017)
- [8] J-PET: L. Raczyński et al., *Phys. Med. Biol.* 62, 5076 (2017)

Developing new routine for processing two-dimensional coincidence Doppler energy spectra.

P.S. Stepanov^{1,*}, S.V. Stepanov² and F.A. Selim¹

¹*Center for Photochemical Sciences, Bowling Green State University, OH, USA*

²*Institute of Theoretical and Experimental Physics, Moscow, Russia*

*email: petrs@bgsu.edu

Coincidence Doppler broadening spectroscopy is a powerful technique to study the electron states in a wide range of materials and characterize defects.

Most of the current techniques implement background subtraction algorithms based on single-dimensional background fitting processes [1]. In current work we developed a new routine for two-dimensional background fitting of the Doppler spectra (Fig. 1). Subtraction of this two-dimensional fit provides a spectrum with more energy pairs related to the same positron-electron annihilation event. This results in improved calculations of the electron momentum distribution.

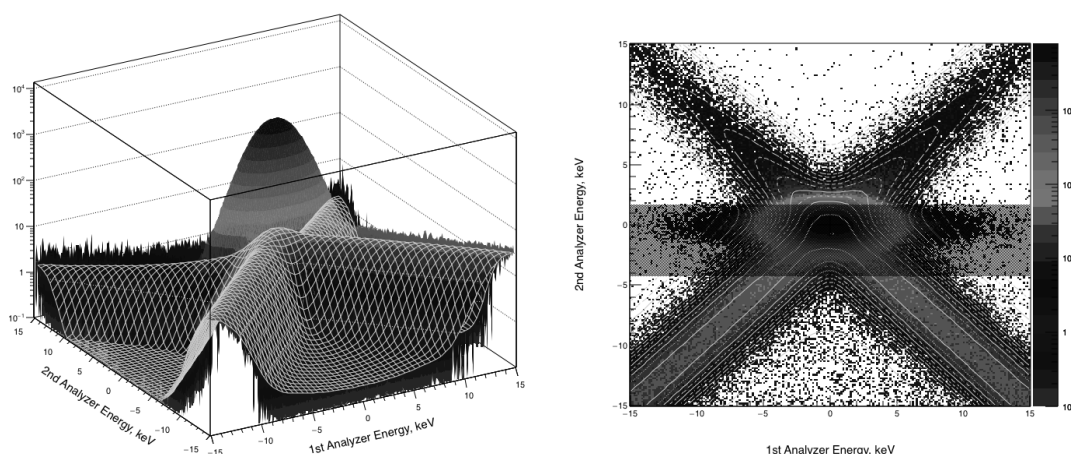


Fig. 1. Background fit of the two-dimensional annihilation energy spectrum of aluminum.

The shape of two-dimensional energy spectrum can be improved if we include contribution of three-gamma annihilation events in the aforementioned background fit.

One-dimensional Doppler spectrum obtained from the 2D histogram should be stretched by the value of a square root of two. Additionally, when calculating S and W parameters from the two-detector Doppler spectrum the integration ranges should be multiplied by a value of two compared to single-detector experiment.

Setting the fitting function of the Doppler spectrum as a sum of parabola and Gaussian functions allows us to estimate the Fermi energy of the material under investigation.

[1] P. Pikart, C. Hugenschmidt, *Nucl. Instrum. Methods Phys. Res., Sect. A*, 750, 61–68 (2014)

P36 | **Effect of the initial microstructure on defect evolution in neutron irradiated Fe-Cr-C alloys**

T. Brodziansky^{1*}, V. Slugeň¹, S. Sojak¹, M. Petriska¹, M.J. Konstantinović²

¹*Institute of Nuclear and Physical Engineering, Faculty of Electrical Engineering and Information Technology, Slovak University of Technology in Bratislava, Ilkovičova 3, 812 19 Bratislava, Slovak Republic*

²*Studiecentrum voor Kernenergie/Centre d'Etude de l'Energie Nucléaire (SCK·CEN), Boeretang 200, B-2400 Mol, Belgium*

*email: tomas.brodziansky@stuba.sk

The irradiation-induced evolution of vacancy type defects in various iron-chromium model alloys and high chromium ferritic/martensitic steels have been studied using coincidence Doppler broadening spectroscopy. Specimens were neutron irradiated to 0.11 dpa at two different temperatures, 300°C and 450°C. It has been found that the microstructure (ferrite vs. ferrite/martensite), more precisely distribution of dissolved carbon within the matrix is one of the key factor that affect response of the materials to neutron irradiation. Presence of dissolved carbon within the matrix leads to formation of stable and immobile carbon-vacancy complexes which act as traps for irradiation induced vacancies and therefore, leading to increased formation of vacancy clusters. Impact of carbon-vacancy complexes on defects evolution during neutron irradiation is relevant only for certain irradiation temperatures.

- [1] M.J. Konstantinović, W.V. Renterghem, M. Matijašević, B. Minov, M. Lambrecht, T. Toyama, M. Chiapetto, L. Malerba, *Phys. Stat. Sol. A*, 213/11, 2988 (2016)
- [2] C. Domain, C. Becquart, J. Foct, *Phys. Rev. B* 69, 144112 (2004)
- [3] M. Matijasević, E. Lucon, A. Almazouzi, *J. Nucl. Mater.* 377, 101 (2008)
- [4] V. Slugen, V. Krsjak, W. Egger, M. Petriska, S. Sojak and J. Vetrenikova, *J. Nucl. Mater.* 409, 163 (2011)

Positron annihilation in magnetite nanopowders prepared by co-precipitation method

K. Durak¹, M. Wiertel^{1,*} and Z Surowiec¹

¹*Department of Nuclear Methods, Faculty of Mathematics, Physics and Computer Science, Maria Curie-Skłodowska University, 1 M. Curie-Skłodowska Sqr., 20-031 Lublin, Poland*

*email: marek.wiertel@umcs.pl

Nanosized iron oxide powders are materials considered with regard to its application in medical therapy called hyperthermia [1]. Magnetite nanopowders with crystallite size varying from 6.6 to 11.8 nm have been prepared by the co-precipitation method [2]. In this study a change of a crystallite size is driven mainly by varying of initial pH of water ammonia solution in which a process of magnetite precipitation runs.

Crystallographic structure and phase composition obtained samples and the size of magnetite nanoparticles were determined by XRD method using Cu K_α radiation. Mössbauer measurements confirmed that nanosized Fe₃O₄ free-flowing powders with sizes above 10 nm are superparamagnetic at room temperature.

Positron lifetime spectroscopy (PALS) has been used to assess defectiveness of microstructure. Experimental PALS spectra were successfully resolved into three lifetime components. The third component ($\tau_3 \approx 1.6$ ns, $I_3 \approx 0.2$ %) can be assigned to a process of *pick-off* annihilation of o-Ps formed in free space between powder particles and due to small intensity is excluded from further discussion of results. Lifetime of positron annihilating from delocalized state in perfect bulk material derived from two-state trapping model [3]:

$$\tau_b = \frac{\tau_1 \cdot \tau_2}{I_2 \cdot \tau_1 + I_1 \cdot \tau_2}, \quad (1)$$

could be determined only for reference bulk magnetite (Alfa Aesar, $d_c = 44$ μm). In all Fe₃O₄ nanopowder samples positron trapping achieves saturation, as a consequence of very high defect concentration. Two types of defects were revealed in the samples with nanometric size of grains. To the first one vacancy clusters in grain insides belongs. The second category of defects is composed of larger vacancy clusters in intergrain boundaries. In a table below the PALS parameters for bulk reference sample and for sample with the crystallite size of 10 nm are shown.

Table 1. PALS parameters for nanosized Fe₃O₄ powders.

Sample	τ_1 [ps]	I_1 [%]	τ_2 [ps]	I_2 [%]	τ_b [ps]	τ_m [ps]
Bulk Fe ₃ O ₄ magnetite large	142.5(8)	66.72(87)	289.0(2.6)	32.80(70)	173.3(8)	193.2(1)
S3, $d_c=10$ nm	265.8(8.5)	22.6(2.8)	424.5(3.7)	77.2(2.7)	not determ.	391.1(3)

Contrary to the PALS results in other nanocrystalline ferrites prepared as compacted powders [4] a lifetime of positron annihilation from delocalized state shortened by positron trapping in defects is not observed in annihilation spectra of nanosized Fe₃O₄ powders.

[1] B. Chudzik, A. Miaskowski, Z. Surowiec, G. Czernel, T. Duluk, A. Marczuk, M. Gagoś, *Int. J. Hyperther.* 32, 842 (2016).

[2] Maryam Tajabadi, Mohammad E. Khosroshahi, *MAPCBEE Proc.* 3, 140 (2012)

[3] A. Seeger, *Appl. Phys.* 4, 183 (1974)

[4] S. Bandyopadhyay, A. Roy, D. Das, S. S. Ghugre and J. Ghose, *Philos. Mag.* 83, 765 (2003)

Dominant defects in hydrogen-embrittled iron detected by positron annihilation spectroscopy

A. Nozaki^{1*}, A. Komatsu¹, K. Koizumi¹, L. Chiari¹ and M. Fujinami¹

¹*Department of Applied Chemistry, Chiba University, 1-33 Yayoi, Inage 263-8522, Japan.*

*email: a.nozaki@chiba-u.jp

It is well known that hydrogen leads to embrittlement in various metals, so that it is very important to clarify the origin of this mechanical degradation. Thermal desorption spectroscopy (TDS) has been often applied to study the defects induced in α -iron by hydrogen embrittlement (HE) and the critical defects are attributed to be the peak at 373 K [1], although its assignment has not been done yet. Positrons are highly sensitive to open-volume type defects. In this work the defects that give rise to hydrogen embrittlement in α -iron have been examined by positron annihilation lifetime spectroscopy (PALS). In a previous study a long lifetime (>300 ps) corresponding to the presence of vacancy clusters appeared in PALS measurements of α -iron strained in a hydrogen environment, although those vacancies hardly form without hydrogen [2]. It has been reported that the susceptibility to hydrogen embrittlement strongly depends on the strain rate. It means that the diffusion of hydrogen is related to hydrogen embrittlement, so that we expect hydrogen-vacancy complexes as the crucial defects in HE. Hence, we have investigated the defect dependence on the strain rate in α -iron and tried to elucidate the crucial defects by measuring the temperature dependence of the positron annihilation spectra from 170 K to 520 K.

The positron lifetime vs. temperature dependence for the slow-strained sample is shown in Fig. 1. The longest lifetime due to vacancy clusters increased gradually from 250 K to 370 K. The induced hydrogen-vacancy complexes released hydrogen, and, as a result, the remaining monovacancies became mobile. That is why the vacancy clusters become larger from 250 K to 370 K. On the contrary, HE was not observed in the fast-strained sample: the longest lifetime corresponding to the vacancy cluster remained constant until 300 K and increased at 315 K, indicating that there were no mobile vacancies below 300 K. From these results, it can be concluded that the vacancy-hydrogen complexes are the crucial defects in α -iron in HE.

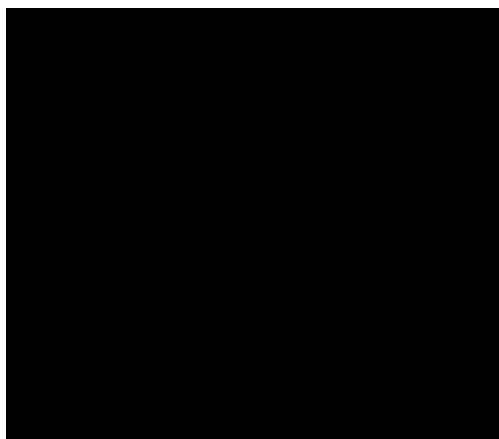


Fig.1 Positron lifetime dependence on temperature for slow-strained iron during the H charge.

[1] K. Takai *et al. Acta Materialia* 56, 5158 (2008)

[2] K. Sakaki *et al. Scr. Mater.* 55, 1031 (2006)

P39 | **Estimate the crystallite size for nanocrystalline AISI 316L stainless steel and Armco iron processed by hydrostatic extrusion using variable energy positron beam**

M. Sarnek^{1*}, E. Dryzek², P. Horodek^{2,3}, W. Pachla⁴

¹ *Cracow University of Economics, Rakowicka 27, 31-510 Kraków, Poland*

² *Institute of Nuclear Physics, Polish Academy of Sciences, E. Radzikowskiego 152, 31-342 Kraków, Poland*

³ *Joint Institute for Nuclear Research, 6 Joliot Curie Str., 141980 Dubna, Russia*

⁴ *Institute of High Pressure Physics, Polish Academy of Sciences (Unipress), Sokołowska 29, 01-142 Warszawa, Poland*

*e-mail: sarnekm@uek.krakow.pl

The paper presents the results of research of nanocrystalline AISI 316L type stainless steel and nanocrystalline Armco pure iron processed by severe plastic deformation using hydrostatic extrusion method. Surface and subsurface of the steel samples extruded at different pressure were investigated using variable energy positron beam. It enabled us to determine the positron diffusion length and compare its values with those for annealed AISI 304 stainless steel. Furthermore positron lifetimes and microhardness were measured for all the samples and X-ray diffraction was used to estimate the crystallite size.

Key words: stainless steel, Armco iron, plastic deformation, hydrostatic extrusion, variable energy positron beam, X-ray diffraction

P40 | Impact of impulse shot peening parameters on properties of stainless steel surface

Marek Wiertel¹, Kazimierz Zaleski², Marek Gorgol¹, Agnieszka Skoczylas¹,
Radosław Zaleski^{1,*}

¹ *Institute of Physics, Maria Curie-Skłodowska University, pl. M. Curie-Skłodowskiej 1, 20-031 Lublin, Poland*

² *Faculty of Mechanical Engineering, Lublin University of Technology, ul. Nadbystrzycka 36, 20-618 Lublin, Poland*

*email: radek@zaleski.umcs.pl

Shot peening (SP), a finishing method for machine elements, was applied to austenitic stainless steel (SS) EN 1.4541. SP was performed at various impact energies (E), impact densities (j) and ball diameters (D). Changes in the surface layer caused by SP result in its improved microhardness, which increases monotonically with the increase of E , j and $1/D$. However, its changes with E and j achieves saturation at about 400 HV0.5. In contrary, no saturation is observed in the investigated range for $1/D$.

Our previous studies have shown the properties of unalloyed, bearing and carburizing steels, and aluminum and titanium alloys can be connected to the microstructure of the surface layer revealed by positron annihilation lifetime spectroscopy (PALS) [1,2]. Therefore, the same approach was applied to the stainless steel EN 1.4541. In the un-shot peened 1.4541 SS, lifetime component corresponding to the positron annihilation from delocalized state of positrons in bulk was found. Its lifetime (86 ps) is shortened due to positron trapping in defects, which are represented by the second component with lifetime (164 ps) suggesting that among the defects predominate vacancies on the edge dislocations. In the shot peened 1.4541 SS samples the bulk component is no longer observed. Instead, two types of defects can be identified: vacancy-like defects coupled with edge dislocations (150 ps) and monovacancies or their small clusters (180-190 ps).

In contrary to our previous studies, PALS and hardness testing results do not correspond very well. The most probable reason for this are different depth profiles of both methods. It seems that the defects, which are responsible for the increase of static microhardness above 400 HV0.5 are located mostly below the surface layer penetrated by positrons.

[1] R. Zaleski, K. Zaleski, M. Gorgol and M. Wiertel. *Applied Physics A* **120**, 551-559 (2015).

[2] R. Zaleski, M. Gorgol and K. Zaleski. *Physics Procedia* **35**, 92-97 (2012).

P41 | **Cardiac myxoma studies with Positron Annihilation Lifetime Spectroscopy**

E. Kubicz^{1,*}, G. Grudzień^{2,3} on behalf of the J-PET collaboration

¹*Institute of Physics, Jagiellonian University, Kraków*

²*Department of Cardiovascular Surgery and Transplantology, Collegium Medicum,
Jagiellonian University, Krakow*

³*John Paul II Specialist Hospital, Krakow*

*email: ewelina.kubicz@doctoral.uj.edu.pl

Positron Annihilation Lifetime Spectroscopy (PALS) allow to examine structure of materials at nano and sub-nanometer level. This technique is based on the lifetime and production intensity of ortho-positronium atoms in free volumes of given structures. Mostly it has an application in studies of organic material, but it can also be used for studies and morphometric imaging as proposed in patent [1]. Some studies performed e.g. by group of Y. C. Jean [2-4], shows that morphology of cells is correlated with the PALS parameters.

Previous studies conducted by the J-PET collaboration of model micro-organisms, e.g. *Saccharomyces cerevisiae* both with dry and aqueous samples allowed to determine the correlation between hygroscopicity of the cell and PALS parameters [5-6]. This experiment proved that PALS can be successfully used for studies of living organisms their dynamics and its relation to the cells morphology.

In this poster preliminary results of studies with Cardiac Myxoma tumor will be presented. This study is a first step on a way to develop imaging of positronium properties produced in the human body during the PET examination. For this aim J-PET group develop detector [8-10] and dedicated reconstruction methods [11-12].

[1] P. Moskal et al, Patent Application No.: P 405185, PCT/EP2014/068374

[2] Y. C. Jean et al, *Applied Surface Science* 252, 3166–3171 (2006)

[3] G. Liu et al, *Phys. stat. sol. (c)* 4, No. 10 (2007)

[4] G. Liu et al, *Applied Surface Science* 255, 115–118 (2008)

[5] B. Jasińska et al, *Acta Phys. Polon. B* 47, 453 (2016)

[6] E. Kubicz et al, *Nukleonika* 60, 749 (2015)

[8] P. Moskal, N. Zoń et. al, *Nucl. Instr. and Meth. A* 775, 54 – 62 (2015)

[9] P. Moskal et al, *Phys. Med. Biol.* 61, 2025-2047 (2016)

[10] L. Raczyński et al, *Nucl. Instr. and Meth. A* 786, 105-112 (2015)

[11] D. Kamińska et al. *Eur. Phys. J. C* 76:445 (2016)

[12] A. Gajos et al. *Nucl. Instr. and Meth. A* 819, 54-59 (2016)

P42 | Study the linear polarization of the positron and positronium by using the J-PET detector

Muhsin Mohammed^{1,10,*}, Aleksander Gajos¹, Daria Kaminska¹, Dominika Alfs¹, Piotr Bialas¹, Catalina Curceanu³, Eryk Czerwinski¹, Andrzej Danel⁴, Kamil Dulski¹, Bartosz Glowacz¹, Marek Gorgol⁵, Beatrix Hiesmayr⁶, Bozena Jasinska⁵, Krzysztof Kacprzak¹, Andrzej Kochanowski⁷, Grzegorz Korcyl¹, Pawel Kowalski⁸, Tomasz Kozik¹, Wojciech Krzemien⁹, Ewelina Kubicz¹, Mateusz Kucharek⁴, Monika Pawlik-Niedzwiecka¹, Szymon Niedzwiecki¹, Marek Palka¹, Lech Raczynski⁸, Zbigniew Rudy¹, Oleksandr Rundel¹, Neha G. Sharma¹, Michal Silarski¹, Tomasz Uchacz⁷, Anna Wieczorek^{1,2}, Wojciech Wislicki⁸, Bozena Zgardzinska⁵, Marcin Zielinski¹, Pawel Moskal¹

¹ *Faculty of Physics, Astronomy and Applied Computer Science, Jagiellonian University, 30-348 Krakow, Poland*

² *Institute of Metallurgy and Materials Science of Polish Academy of Sciences, 30-059 Krakow, Poland*

³ *INFN, Laboratori Nazionali di Frascati, 00044 Frascati, Italy.*

⁴ *Institute of Chemistry and Physics, University of Agriculture, 30-149 Krakow, Poland*

⁵ *Institute of Physics, Maria Curie-Skłodowska University, 20-031 Lublin, Poland.*

⁶ *Faculty of Physics, University of Vienna, 1090 Vienna, Austria*

⁷ *Faculty of Chemistry, Jagiellonian University, 30-060 Krakow, Poland*

⁸ *Department of Complex System, National Centre for Nuclear Research, 05-400 Otwock-Swierk, Poland*

⁹ *High Energy Physics Division, National Centre for Nuclear Research, 05-400 Otwock-Swierk, Poland*

¹⁰ *Department of Physics, College of Education for Pure Sciences, University of Mosul, Mosul, Iraq*

* email: muhsin.m@doctoral.uj.edu.pl

A method for measuring the linear polarization of positron and ortho positronium (o-Ps) atom is proposed which is based on the determination of the angular distribution of the normal to the decay plane with respect to the o-Ps spin orientation. In the case of the linear polarization we can determine it on the event by event basis as a direction of the positron motion. The unique geometry and properties of the J-PET enables to design the positron source such that the linear polarization of produced o-Ps can be determined. Due to the parity violation in the beta decay the emitted positrons are longitudinally polarized with the polarization vector equal to $p = v/c$, where v denotes the positron velocity, c is the speed of light. The J-PET is a novel tomography device using plastic polymer instead of conventional crystal. It can be used to study the Ps polarization, we can also study the degree of the o-Ps polarization which may be monitoring based on the measurements of the angular distribution between the normal to the 3γ decay plane and the o-Ps spin direction.

P43 | **Human tissue investigations using PALS technique – free radicals influence**

B. Jasińska^{1,*}, B. Zgardzińska¹, G. Chołubek², M. Pietrow¹, M. Gorgol¹, K. Wysogład¹,
H. Wiktor², K. Wiktor², P. Białas³, C. Curceanu⁶, E. Czerwiński³, K. Dulski³, A. Gajos³,
B. Głowacz³, B. Hiesmayr⁷, D. Kamińska³, G. Korcyl³, P. Kowalski⁴, T. Kozik³,
N. Krawczyk³, W. Krzemień⁵, E. Kubicz³, M. Mohammed^{3,8}, M. Pawlik-Niedźwiecka³,
S. Niedźwiecki³, M. Pałka³, L. Raczyński⁴, Z. Rudy³, N. G. Sharma³, S. Sharma³,
M. Silarski³, M. Skurzok³, A. Wieczorek³, W. Wiślicki⁴, M. Zieliński³, P. Moskal³

¹ *Institute of Physics, Maria Curie Skłodowska University, Pl. Marii Curie Skłodowskiej 1,
20-031 Lublin, Poland*

² *Medical University of Lublin, Aleje Raławskie 1, 20-950 Lublin*

³ *Faculty of Physics, Astronomy and Applied Computer Science, Jagiellonian University,
30-348 Cracow, Poland*

⁴ *Department of Complex Systems, National Centre for Nuclear Research,
05-400 Otwock-Świerk, Poland*

⁵ *High Energy Physics Division, National Centre for Nuclear Research,
05-400 Otwock-Świerk, Poland*

⁶ *INFN, Laboratori Nazionali di Frascati, 00044 Frascati, Italy*

⁷ *Faculty of Physics, University of Vienna, 1090 Vienna, Austria*

⁸ *Department of Physics, College of Education for Pure Sciences, University of Mosul, Mosul,
Iraq*

*email: bozena.jasinska@poczta.umcs.lublin.pl

The Positron Annihilation Lifetime Spectroscopy (PALS) was applied to the samples which were the uterine leiomyomata human tissue and the normal tissue taken from an adequate place. The method indicated differences in values of the measured PALS parameters for both types of samples. These differences are related mainly to free radicals which were present in both tissues. The measurements were performed either in darkness and in presence of visible light which influenced the radicals and, as a result, made changes in PALS parameters values.

[1] Y.C. Jean et al., J Am Chem Soc. 99 (1977) 1623.

[2] G. Liu, H. Chen, L. Chakka, J. E. Gadzia, and Y. C. Jean., Phys. Stat. Sol. (c) 10 (2007) 3912.

[3] Y.C. Jean et al., Applied Surface Science 252 (2006) 3166.

[4] E. Axpe et al., PLoS One 2 (2014) 83838.

[5] C. Hugenschmidt and H. Ceeh, J. Phys. Chem. B 118 (2014) 9356.

[6] E. Kubicz et al., Nukleonika 60 (2015) 749.

[7] P. Moskal et al., Nucl. Inst. and Meth. A 764 (2014) 317.

[8] P. Moskal et al., Patent Application: P 405185 (2013), PCT/EP2014/068374 (2014), WO2015028604.

[9] B. Jasińska et al., *Human tissues investigation using PALS technique*, submitted to Acta Phys. Polon. B (2017).

Alphabetical list of participants with the contact details					
No	Name	Surname	E-mail	Institution	City, country
1	Yulia	Akmalova	AkmalovaYuliya@gmail.com	National Research Nuclear University MEPhI	Moscow, Russia
2	Ashraf	Alam	m.a.alam@bristol.ac.uk	University of Bristol	Bristol, England
3	Nikolay	Arutyunov	n_arutyunov@yahoo.com	1) Martin Luther University Halle-Wittenberg, 2) Institute of Electronics	1) Halle, Germany, 2) Tashkent, Uzbekistan
4	Ahmed	Attallah	agamal86_physics@yahoo.com	Martin Luther University Halle-Wittenberg	Halle, Germany
5	Josef	Bartoš	Jozef.Bartos@savba.sk	Polymer Institute of Slovak Academy of Sciences	Bratislava, Slovakia
6	Artur	Błażewicz	artur.blazewicz@poczta.umcs.lublin.pl	Maria Curie-Skłodowska University	Lublin, Poland
7	Tomáš	Brodziansky	tomasbrodziansky@gmail.com	Slovak University of Technology of Bratislava	Bratislava, Slovakia
8	Roberto	Brusa	brusa@science.unitn.it	University of Trento	Trento, Italy
9	Mieczysław	Budzyński	budzyn@poczta.umcs.lublin.pl	Maria Curie-Skłodowska University	Lublin, Poland
10	Maik	Butterling	m.butterling@hzdr.de	Helmholtz-Zentrum Dresden-Rossendorf	Dresden, Germany
11	Xingzhong	Cao	caoxzh@ihep.ac.cn	Institute of High Energy Physics of the Chinese Academy of Sciences	Beijing, China
12	Yuanyuan	Cao			Wuhan, China
13	David	Cassidy	d.cassidy@ucl.ac.uk	University College London	London, England
14	Katarína	Čechová	katarina.cechova@savba.sk	Slovak Academy of Sciences	Bratislava, Slovakia
15	Shivani	Choudhary	shivanihdhr6@gmail.com	Jagiellonian University	Cracow, Poland
16	Jakub	Čížek	jakub.cizek@mff.cuni.cz	Charles University	Prague, Czech Republic
17	Giovanni	Consolati	giovanni.consolati@polimi.it	Politecnico di Milano	Milan, Italy
18	Doru	Dinescu	doru.dinescu@eli-np.ro	Horia Hulubei National Institute for Physics and Nuclear Engineering	Bucharest, Romania
19	Ewa	Dryzek	ewa.dryzek@ifj.edu.pl	Institute of Nuclear Physics of Polish Academy of Sciences	Cracow, Poland
20	Jerzy	Dryzek	jerzy.dryzek@ifj.edu.pl	Institute of Nuclear Physics of Polish	Cracow, Poland

				Academy of Sciences	
21	Leonid	Dubov	lydubov@mephi.ru	National Research Nuclear University MEPhI	Moscow, Russia
22	Kamil	Dulski	kamil.dulski@gmail.com	Jagiellonian University	Cracow, Poland
23	Katarzyna	Durak	kasiadur@wp.pl	Maria Curie-Sklodowska University	Lublin, Poland
24	Werner	Egger	werner.egger@unibw.de	Universität der Bundeswehr München	Neubiberg, Germany
25	Pengfei	Fang	fangpf@whu.edu.cn	Wuhan University	Wuhan, China
26	Kamil	Fedus	kamil@fizyka.umk.pl	Nicolaus Copernicus University	Toruń, Poland
27	Mirosław	Fordon	m.fordon@uni-export.com.pl	UNI-EXPORT INSTRUMENTS POLSKA	Warsaw, Poland
28	Jan	Franz	jfranz@mif.pg.gda.pl	Gdansk University of Technology	Gdańsk Poland
29	Masanori	Fujinami	fujinami@faculty.chiba-u.jp	Chiba University	Chiba, Japan
30	Naoko	Fujinami			Chiba, Japan
31	Mahmoud	Gomaa	mahmoud_gomaa19@mu.edu.eg	Technische Universität München	Garching, Germany
32	Marek	Gorgol	marek.gorgol@poczta.umcs.lublin.pl	Maria Curie Sklodowska University	Lublin, Poland
33	Tomasz	Goworek	tomasz.goworek@poczta.umcs.lublin.pl	professor emeritus, Maria Curie Sklodowska University	Lublin, Poland
34	Chunqing	He	hecq@whu.edu.cn	Wuhan University	Wuhan, China
35	Tetsuya	Hirade	t.hirade@kurenai.waseda.jp	Japan Atomic Energy Agency	Tsukuba, Japan
36	Petr	Hruska	peta.hruska.l@gmail.com	Charles University	Prague, Czech Republic
37	Toshio	Hyodo	hyodot@post.kek.jp	High Energy Accelerator Research Organization (KEK)	Tsukuba, Japan
38	Shoji	Ishibashi	shoji.ishibashi@aist.go.jp	National Institute of Advanced Science and Technology (AIST)	Tsukuba, Japan
39	Yuki	Ishibashi			Tsukuba, Japan
40	Kenji	Ito	k-ito@aist.go.jp	National Institute of Advanced Science and Technology (AIST)	Tsukuba, Japan
41	Mio	Ito			Tsukuba, Japan
42	Bożena	Jasińska	bozena.jasinska@poczta.umcs.lublin.pl	Maria Curie-Sklodowska University	Lublin, Poland
43	Łukasz	Kapłon	lukasz.kaplon@doctoral.uj.edu.pl	Jagiellonian University	Cracow, Poland

44	Grzegorz	Karwasz	karwasz@fizyka.umk.pl	Nicolaus Copernicus University	Toruń, Poland
45	Taras	Kavetskyy	kavetskyy@yahoo.com	The John Paul II Catholic University of Lublin	Lublin, Poland
46	Grzegorz	Korcyl	grzegorz.korcyl@uj.edu.pl	Jagiellonian University	Cracow, Poland
47	Reinhard	Krause-Rehberg	reinhard.krause-rehberg@physik.uni-halle.de	Martin Luther University Halle-Wittenberg	Halle, Germany
48	Vladimir	Krsjak	vladimir.krsjak@stuba.sk	Slovak University of Technology	Bratislava, Slovakia
49	Ewelina	Kubicz	ewelina.kubicz@doctoral.uj.edu.pl	Jagiellonian University	Cracow, Poland
50	Jan	Kuriplach	Jan.Kuriplach@mff.cuni.cz	Faculty of Mathematics and Physics, Charles University	Prague, Czech Republic
51	Yoshihiro	Kuzuya	kuzuya.yoshihiro.52e@st.kyoto-u.ac.jp	1) Kyoto University, 2) National Institute of Advanced Science and Technology (AIST)	1) Osaka, Japan 2) Ibaraki, Japan
52	Roman	Laptev	laptevrs@tpu.ru	National Research Tomsk Polytechnic University	Tomsk, Russia
53	Andrey Markovich	Lider	lider@tpu.ru	National Research Tomsk Polytechnic University	Tomsk, Russia
54	Maciej Oskar	Liedke	m.liedke@hzdr.de	Helmholz-Zentrum Dresden-Rossendorf	Dresden, Germany
55	Ilja	Makkonen	ilja.makkonen@aalto.fi	Aalto University	Aalto, Finland
56	Oksana	Melikhova	Oksana.Melikhova@mff.cuni.cz	Charles University	Prague, Czech Republic
57	Koji	Michishio	koji.michishio@aist.go.jp	National Institute of Advanced Industrial Science and Technology (AIST)	Tsukuba, Japan
58	Izumi	Mochizuki	mochizu@post.kek.jp	High Energy Accelerator Research Organization (KEK)	Tsukuba, Japan
59	Hamdy FM	Mohamed	hamdyfm@gmail.com	Minia University	Minia, Egypt
60	Muhsin	Mohammed	muhsin.m@doctoral.uj.edu.pl	Jagiellonian University	Cracow, Poland
61	Paweł	Moskal	p.moskal@uj.edu.pl	Jagiellonian University	Cracow, Poland
62	Szymon	Niedźwiecki	szymon.niedzwiecki@uj.edu.pl	Jagiellonian University	Cracow, Poland
63	Madoka	Nippa	madoka.nippa@chiba-u.jp	Chiba University	Chiba, Japan

64	Ludmila	Nikitina	nikitina@tpu.ru	National Research Tomsk Polytechnic University	Tomsk, Russia
65	Ayaka	Nozaki	a.nozaki@chiba-u.jp	Chiba University	Chiba, Japan
66	Brian	ORourke	brian-orourke@aist.go.jp	National Institute of Advanced Industrial Science and Technology (AIST)	Tsukuba, Japan
67	Monika	Pawlik-Niedźwiecka	monika.pawlik@doctoral.uj.edu.pl	Jagiellonian University	Cracow, Poland
68	Somayeh	Payedarfard			
69	Marek	Pietrow	mrk@kft.umcs.lublin.pl	Maria Curie-Skłodowska University	Lublin, Poland
70	Ivan	Prochazka	ivan.prochazka@mff.cuni.cz	Charles University	Prague, Czech Republic
71	Anita	Pujari			Mumbai, India
72	Pradeep Kumar	Pujari	pujari@barc.gov.in	Bhabha Atomic Research Centre	Mumbai, India
73	Juhi	Raj	juhi.nagaraj@gmail.com	Jagiellonian University	Cracow, Poland
74	Hasi	Ray	hasi_ray@yahoo.com	Study Center JnganSikha & New Alipore College Kolkata	Kolkata, India
75	Nagisa	Sakata	nagisa.sakata@chiba-u.jp	Chiba University	Chiba, Japan
76	Maciej	Sarnek	sarnekm@uek.krakow.pl	Cracow University of Economics	Cracow, Poland
77	Matúš	Saro	matus.saro@stuba.sk	Slovak University of Technology	Bratislava, Slovakia
78	Jan	Sarzyński	sarzyn@hektor.umcs.lublin.pl	emeritus, Maria Curie-Skłodowska University	Lublin, Poland
79	Ondrej	Šauša	ondrej.sausa@savba.sk	Slovak Academy of Sciences	Bratislava, Slovakia
80	Farida	Selim	faselim@bgsu.edu	Bowling Green State University	Bowling Green, USA
81	Victor	Shantarovich	shant@center.chph.ras.ru	Institute of Chemical Physics Russian Academy of Sciences	Moscow, Russia
82	Sushil	Sharma	sushil.sharma@uj.edu.pl	Jagiellonian University	Cracow, Poland
83	Michał	Silarski	michal.silarski@uj.edu.pl	Jagiellonian University	Cracow, Poland
84	Magdalena	Skurzok	mskurzok@gmail.com	Jagiellonian University	Cracow, Poland
85	Vladimir	Slugen	vladimir.slugen@stuba.sk	Slovak University of Technology	Bratislava, Slovakia

86	Anna	Slugen			Bratislava, Slovakia
87	Sergey	Stepanov	stepanov@itep.ru	Institute of Theoretical and Experimental Physics	Moscow, Russia
88	Zbigniew	Surowiec	zbigniew.surowiec@umcs.pl	University of Maria Curie-Sklodowska	Lublin, Poland
89	Helena	Švajdlenková	upolhela@savba.sk	Polymer Institute of Slovak Academy of Sciences	Bratislava, Slovakia
90	Takayuki	Tachibana	tachibana@rs.tus.ac.jp	Tokyo University of Science	Tokyo, Japan
91	Masanori	Tachikawa	tachi@yokohama-cu.ac.jp	Yokohama City University	Yokohama, Japan
92	Giacomo	Tanzi	giacomo.tanzi@unimi.it	University of Milan	Milan, Italy
93	J. David	Van Horn	vanhornj@umkc.edu	University of Missouri-Kansas City	Kansas City, USA
94	Baoyi	WANG	wangboy@ihep.ac.cn	Institute of High Energy Physics of the Chinese Academy of Sciences	Beijing, China
95	Paweł	Warchoł	pawel@irtech.pl	IRtech Sp. z o.o.	Cracow, Poland
96	Jan	Wawryszczuk	jan@poczta.umcs.lublin.pl	emeritus, Maria Curie-Sklodowska University	Lublin, Poland
97	Marek	Wiertel	marek.wiertel@poczta.umcs.lublin.pl	Maria Curie-Sklodowska University	Lublin, Poland
98	Konrad	Wysogład	konrad1274@gmail.com	Maria Curie-Sklodowska University	Lublin, Poland
99	Shigeru	Yoshimoto	Shigeru_Yoshimoto@trc.toray.co.jp	Toray Research Center, Inc	Otsu, Japan
100	Radek	Zaleski	radek@zaleski.umcs.pl	Maria Curie-Sklodowska University	Lublin, Poland
101	Bożena	Zgardzińska	bozena.zgardzinska@poczta.umcs.lublin.pl	Maria Curie-Sklodowska University	Lublin, Poland