Book of abstracts

Sixteenth International Workshop
on **Slo**w **Pos**itron Beam Techniques and Applications

Orléans, 16-21th July 2023

SLOPOS-16, the sixteenth International Workshop on Slow Positron Beam Techniques and applications, will be held from 16-21thJuly 20023 in Orléans, France. The aim of the workshop is to provide an opportunity for exchange of the latest results and scientific information concerning the positron interactions with solids and surfaces, the generation of slow positron beams and their applications.

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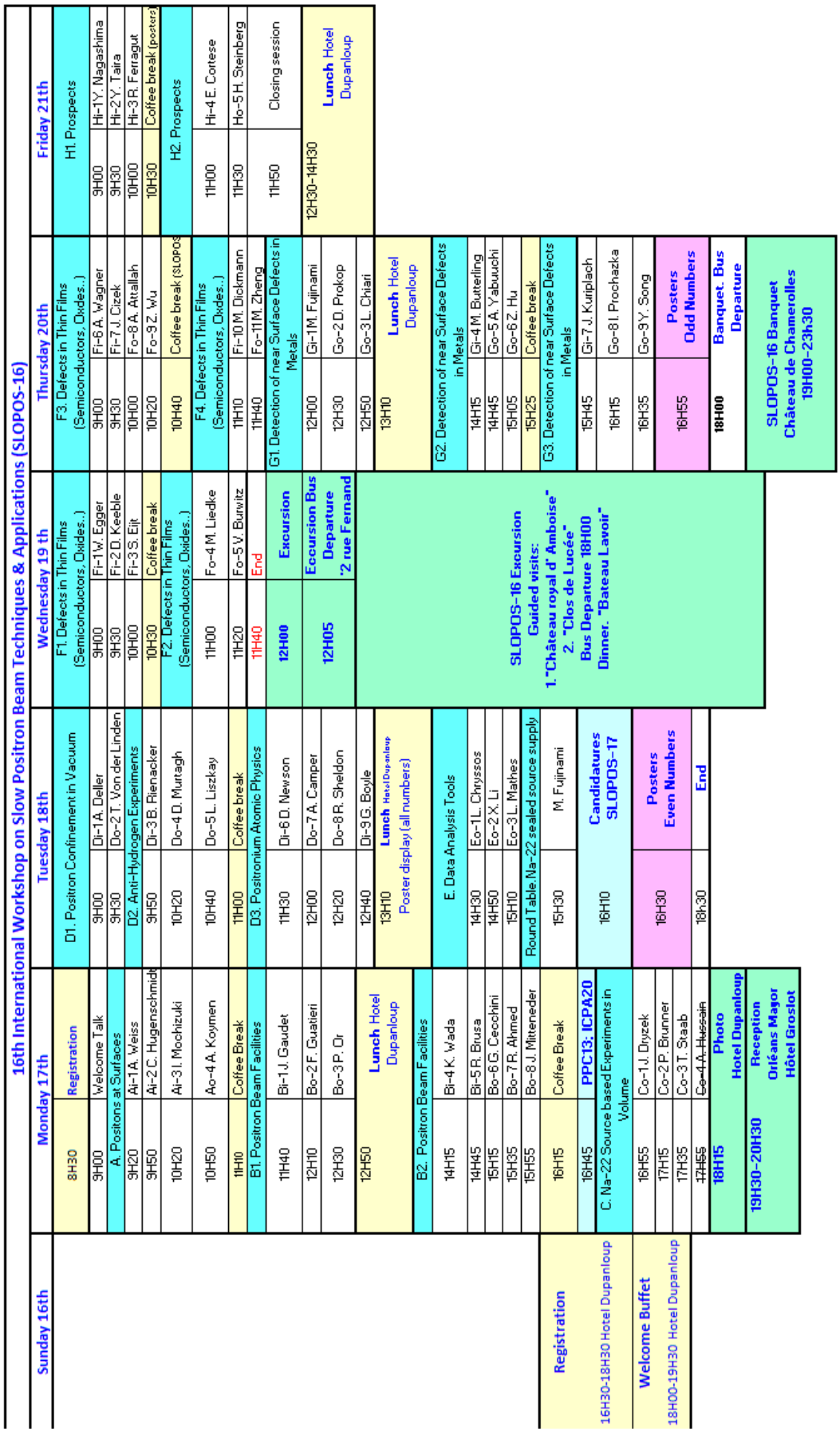
Main Topics of the workshop

- Positron/Positronium interaction at surfaces and in near surface (≤ 1.0(5) μm)
- Positron/Positronium annihilation spectroscopy at surfaces and in near surface
- Low Energy positron Beams: continuous, pulsed, high intensity
- Positon Traps & Microscope
- Positron/Positronium diffraction, scattering, transport and reemission
- Positronium atomic physics
- Positron trapping and defect profiling in near surface
- Defect and electrical field at interfaces
- Ps trapping and nanopores profiling in near surface
- Theory; Calculations of annihilation characteristics
- Gas, liquids, solids

Invited speakers

Boyle Gregory	James Cook University, AUSTRALIA
Brusa Roberto	University of Trento & TIFPA/INFN , ITALY
Butterling Maik	HZDR, GERMANY
Cizek Jakub	Charles University, CZECH REPUBLIC
Cortese Erika	University of Southampton, UK
Deller Adam	Max Planck IPP, GERMANY
Dickmann Marcel	Universität der Bundeswehr, GERMANY
Eijt Stephan	Delft University of Technology, THE NETHERLANDS
Egger Werner	University of the Bundeswehr, GERMANY
Ferragut Rafael	Politecnico di Milano, & INFN, ITALY
Fujinami Masanori	Chiba University, JAPAN
Gaudet James	Mc Master university, CANADA
Hugenschmidt Christoph	MLZ, Technische Universität, GERMANY
Keeble David	University of Dundee, UNITED KINGDOM
Kuriplach Jan	Charles University, CZECH REPUBLIC
Mochizuki Izumi	KEK, JAPAN.
Nagashima Yasuyuki	Tokyo University of Science, JAPAN
Newson Donovan	UCL , UNITED KINGDOM
Rienacker Benjamin	University of Liverpool, UNITED KINGDOM
Taira Yoshitaka	IMS, NINS JAPAN
Wada Ken	KEK, JAPAN
Wagner Andreas	HZDR, GERMANY
Weiss A. H.	University of Texas, USA

Program Overview



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A. Positons at Surfaces

Core Contribution to the Doppler Broadened Annihilation Spectra: Surface vs Bulk

A. H. Weiss[a], S. Lotfimarangloo[a], J. Driscoll[a], R. W. Gladen[a], A. J. Fairchild[a], I. Makkonen[b], B. Barbielllini[c], P. A. Sterne[d], A. R. Koymen[a], and V. A. Chirayath[a]

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Here we report coincidence Doppler broadened spectra (DBS) resulting from the annihilation of positrons bound in a surface state on clean and adsorbate covered surfaces. These spectra are compared with DBS resulting from the annihilation of positrons in bulk states. Our results indicate that the surface does indeed act like a giant open volume defect resulting in a dramatic (of order 50%) reduction of the relative contributions of the core contributions. Figure 1 below shows the DBS spectra resulting from the annihilation of a positron implanted at 21 eV into an image potential state on a clean Cu surface in comparison to the DBS spectra obtained from a positron annihilating after implantation at 21keV. It may be seen that the DBS from the surface is obviously narrower reflecting the reduced core contributions. We will report on this experiment as well as other measurements and theoretical analysis where we fit the measured spectra with DBS obtained from ab-initio methods for the bulk and surface obtained by changing the relative contributions of the model DBS spectra calculated for individual atomic levels.

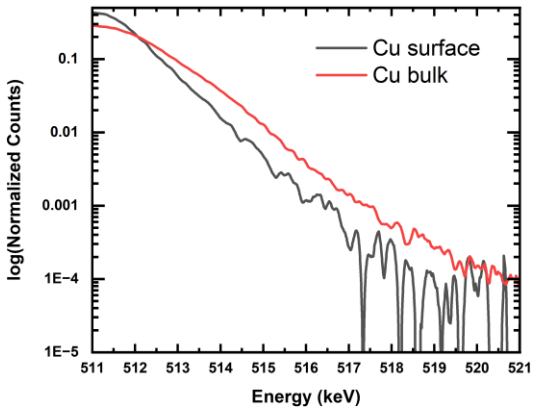

Fig. 1 Comparison of DBS spectra resulting from the annihilation of positrons bound in an image potential state on clean Cu with that obtained from positrons in bulk states in Cu.

Positron Diffraction on Hydrogen-Intercalated Quasi-Free-Standing Graphene on 6H-SiC(0001)

M. Dodenhöft [a], I. Mochizuki[b], K. Wada[b], T. Hyodo[b], P. Richter[c], P. Schädlich[c], T. Seyller[c], and C. Hugenschmidt[a]

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With the advent of bright low-energy positron beams novel analysis tools have been developed exploiting the unique properties of positron matter interaction. Various surface sensitive positron techniques profit from particular features such as the absence of exchange interaction, repulsive crystal potential as well as trapping of thermalized positrons in delocalized surface states [1]. The positron counterpart of electron-based techniques such as reflection high-energy electron diffraction (RHEED) and electron induced Auger-electron spectroscopy (EAES) intrinsically exhibit superior surface sensitivity. In contrast to electrons, positrons show the phenomenon of total reflection for small glancing angles. With total reflection high-energy positron diffraction (TRHEPD) the structure of the topmost and the immediate subsurface atomic layers of surfaces can be revealed with outstanding accuracy [2].
Within this contribution I will focus on recent TRHEPD studies on the structure of hydrogen-intercalated quasi-free-standing monolayer graphene (QFMLG) on 6H-SiC(0001). We performed rocking curve analysis based on the full dynamical diffraction theory to precisely determine the spacing between QFMLG and the SiC substrate. The TRHEPD results are compared with findings obtained by complementary synchrotron-based techniques and calculation results based on density-functional theory (DFT). Finally, I will also give a brief overview of future element- and structure-sensitive surface investigations at the high-intensity positron source NEPOMUC and the implementation of new instrumentation. [3].

[1] C. Hugenschmidt; Surf. Sci. Reports 71 (2016) 547
[2] Y. Fukaya, A. Kawasuso, A. Ichimiya, and T. Hyodo; J. Phys. D: Appl. Phys. 52 (2019) 013002
[3] M. Dodenhöft, S. Vohburger, and C. Hugenschmidt; Rev. Sci. Instrum. 92 (2021) 115103

An effective use of total-reflection high-energy positron diffraction (TRHEPD) for the detection of H atoms: application to H-terminated CeO_2 (111)-1×1 surface

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Recently, hydrogen (H)-terminated ceria (CeO_2) has been attracting much attention as a promotive catalyst for hydrogenation reactions with low activation energy [1] and high reactive efficiency [2], a synthesis-gas production by solar power [3], etc. In order to unravel roles of the H atoms during reactions on the transition-metal dioxide, it is crucial to determine their exact positions.
However, detection of H by X-ray or electron diffraction tecnique is difficult as its scattering factor is smallest due to its smallest atomic number. Neutron scattering techniques are used to detect H atoms in the bulk, but it is very difficult to detect those existing only on the topmost surface.
We are developing a new method for the precise determination of the atomic configuration of H-terminated surfaces by making a novel effective use of the total-reflection high-energy positron diffraction (TRHEPD), which is exceedingly surface-sensitive [4]. The target material is H-terminated CeO_2 (111)-1×1 surface. Even though the scattering amplitude of H is also very small for the positron, we found certain incident azimuthal angles where the rocking curve (glancing angle dependence of the 00-spot intensity) changes sensitively by the presence/absence of the adsorbed H atoms. In this presentation, we show the TRHEPD results with the structral analysis for the H-terminated surface and discuss why the H atom is detectable at the particular incident azimuth conditions.

[1] M. G.-Melchor *et al*., ACS Catal. **4**, 4015 (2014).
[2] S. Zhang *et al*., Nat. Commun. **8**, 15266 (2017).
[3] S. Zoller *et al*., Joule **6**, 1606 (2022).
[4] Y. Fukaya *et al*., J. Phys. D: Appl. Phys. **52**, 013002 (2019).

Positron induced electron spectroscopy of Si (100) surface

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Positron induced electron spectroscopy can provide information on elemental composition [1], electronic structure [2] and throw light on hitherto unobserved electronic transitions [3] from the topmost atomic layers. Here we report on various processes that contribute to electron emission from silicon (100) surface following the impact of a low energy positron. By changing the energy of the implanted positrons from 1.25 eV to 900 eV, we were able to identify low energy electrons emitted via (i) positron annihilation induced Auger emission processes (PAES), (ii) Auger mediated positron sticking (AMPS) and (iii) positron impact induced secondary electron emission (PIISE). By using positrons with energy below the threshold required for AMPS or PIISE, we show the existence of an Auger relaxation process which is initiated by annihilation induced deep valence hole in silicon. It is impossible to measure the spectra of Auger electrons emitted following these Auger (called VVV) transitions using traditional photon-based or electron-based techniques due to the obscuring presence of large probe-induced secondary electron background. We have obtained the efficiency for VVV Auger transition in Si by fitting the VVV Auger spectra and will discuss its implications for device physics using Si. Increasing the energy of positrons above the AMPS threshold, but keeping it below the PIISE threshold, allows the measurement of the electronic structure of the topmost atomic layer of silicon providing a way to investigate variations in surface electronic structure with changes in surface termination. By taking the energy of positrons beyond the PIISE threshold, we obtain the true secondary electron spectrum and their yield from Si without the complications of redistributed primary as is the case with electron impact induced secondaries.

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[2] A. J. Fairchild et al., Phys. Rev. Lett. 129, 106801 (2022).
[3] V. A. Chirayath et al., Nature Communication, 8, 16116 (2017).

B1 : Positron beam facilities

Progress on the McMaster Intense Positron Beam Facility (MIPBF)

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The McMaster Intense Positron Beam Facility (MIPBF) was conceived as a collaborative project between the Department of Engineering Physics and the Department of Nuclear Operations and Facilities at McMaster University to produce a positron beamline user facility at the five-megawatt McMaster Nuclear Reactor (MNR) in the city of Hamilton, Canada. Designed for simplicity, the MIPBF uses a single concave platinum sheet, normal to the axis of the beam, as both converter and moderator. An all-magnetic transport system is used to remove the resulting beam from the reactor beamtube, utilizing an S-bend in the vacuum transport system to select for low-momentum positrons and bypass the neutron beam dump shielding. Simultaneous to the construction of the positron generation/transport system, a stand-alone materials science end-station was fabricated and transported to The University of Western Ontario in London, Canada, for testing prior to installation at McMaster University.

An initial test of the MIPBF resulted in concerns of overheating and necessitated a delay and redesign of some shielding components. The modified system was permanently installed in March of 2023 and easily passed all thermal safety validation tests. Work to optimize the positron beam is currently underway prior to installing the materials science end-station at MNR. This talk will cover the initial design, modifications to, and installation of the MIPBF, as well as plans to modify and enlarge the scope of the facility as the scale of nuclear research at McMaster University increases.

Commercial CMOS sensors as state-of-the-art positron imaging devices.

Francesco Guatieri[a], C.O. Michael Berghold[a], C.O. Vassily Vadimovitch Burwitz[a], C.O. Lucian Mathes[a] and C.O. Christoph P. Hugenschmidt[a]

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For the last three decades, real-time imaging of low energy positron beams has been performed using MCP amplification and phosphor screens. Up to now it was accepted that most low-energy positron beams are not intense enough to be imaged directly without amplification. At the same time, the rise of digital cameras and smartphones has prompted the development of integrated imaging sensors with unprecedented resolution and sensitivity, which are now widely available and cheap. We have investigated whether these commercial sensors could be modified to become real-time imaging devices for low-energy positron beams. Our findings show that not only this is feasible, but that the resulting sensor can outperform current techniques with respect to spatial resolution and detection efficiency.

The SPOT-IL Positron Beam Construction and Its Use for Doppler Broadening Measurement of Annealed Cu

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We report here the successive first operation of the Slow POsitron beam faciliTy in IsraeL (SPOT-IL) at the Hebrew University [1-2]. The beam follows a traditional design, but its unique target cell is designed to allow a combined measurement of DB and sample conductivity, and a Liquid Nitrogen based cooling system, with the flexibility to add more detection options in the future. The beam uses a ^{22}Na source, a Tungsten moderator, and a target cell equipped with a load-lock system for easy sample insertion. The beam energy varies between 0.03 keV and 30 keV.
The detection system consists of two high-purity Germanium detectors, facing each other, allowing low-background Doppler-Broadening (DB) measurements. Event readout is done using a state-of-the-art compact desktop system.
The beam has been successfully tested by using it to characterize annealed Copper (Cu) samples. Four annealed samples were measured at various energies (0.5 keV - 20 keV), the results were fitted using VEPFIT, and show consistent behavior with previous measurements.

[1] Or, Paz et al. "SPOT IL-Slow positron facility in Israel." AIP Conference Proceedings. Vol. 2182. No. 1. AIP Publishing LLC (2019).

[2] Or, Paz et al. “The SPOT-IL Positron Beam Construction and Its Use for Doppler Broadening Measurement of Titanium Thin Films”. arXiv preprint arXiv:2007.05921 (2020).

B2 . Positron beam facilities

Renewal of the slow-positron generation unit and user activities at the IMSS Slow Positron Facility, KEK

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The Slow Positron Facility at the Institute of Materials Structure Science (IMSS), KEK is providing a slow-positron beam generated by a dedicated S-band electron linear accelerator (~50 MeV, ~550 W, 50 Hz).
The slow positron generation unit was renewed in the summer of 2020 with a few modifications. The beam intensity, which had been in the 10^7 slow-e^+/s range in long-pulse (1 μs) mode immediately after the 2010 improvement [1], has been enhanced to 1×10^8 slow-e^+/s.
The long-pulse mode beam is fed to two diffraction experimental stations, the total-reflection high-energy positron diffraction (TRHEPD) [2] and the low-energy positron diffraction (LEPD) [3], while the short-pulse (~10 ns) mode beam is fed to the positronium time-of-flight (Ps-TOF) and the general-purpose stations.
The TRHEPD is a positron version of reflection high-energy electron diffraction (RHEED). The TRHEPD station is increasingly being used by surface scientists and has produced results on surface structural analysis (determining the atomic positions of the surface and immediate subsurface atomic layers).
At the LEPD station, overall improvements to the experimental station have reduced the measurement time by nearly two orders of magnitude compared to the initial experiments [3]. A diffraction pattern of the Cu(001) surface can now be obtained in a matter of minutes, allowing data to be collected at many incident energies for structural analysis on the clean surface before the crystal surface is contaminated. In addition, the sample used for the LEPD measurements was transported to the KEK Photon Factory in an ultra-high vacuum transport vessel to keep the sample surface clean, and angle-resolved photoemission spectroscopy (ARPES) spectra were obtained.
The Ps-TOF station is used to study semiconductor surfaces [4] and Ps-generating materials for Ps cooling experiments. The general-purpose experimental station, which was previously used for positronium negative ion experiments [5], is now being used for Ps laser-cooling experiments.

[1] K. Wada et al., Eur. Phys. J. D 66, 37 (2012).
[2] Y. Fukaya et al., J. Phys. D: Appl. Phys. 52, 013002 (2019).
[3] K. Wada et al., e-J. Surf. Sci. Nanotech. 16, 313 (2018).
[4] A. Kawasuso et al., J. Phys. B: At. Mol. Opt. Phys. 54, 205202 (2021).
[5] K. Michishio et al., Nat. Commun. 7, 11060 (2016).

Bunched positron beams at the AntiMatter Laboratory (AML) in Trento and planned experiments

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The AML of Trento is equipped since many years with a continuous positron beam fully electrostatically transported. This beam is still in use and allows solid state and fundamental studies with positrons and positronium (Ps) [1, 2].

A new set-up to produce intense bunches of positrons ($\sim 10\text{^}5$) with a time duration of 2.5 ns and energy tunable up to 20 keV is under construction [3].

The apparatus consists of a Na22 source with a solid rare gas moderator producing a continuous positron beam that can be switched to provide positrons to two different lines. The first line will be devoted to fundamental studies with Ps while the second line to solid state studies.

In the first line there is a Surko trap followed by a buncher and a sample chamber. A novel non adiabatic extraction from the 700 Gauss magnetic field of the Surko trap is realized with a prebunching. The following buncher and the last electrostatic lenses are designed to focus the positron bunches in a magnetic and electrostatic field free region.

In the second line the positrons will be re-moderated and injected in a pulsed beam for PALS studies.

In this talk, I will: 1) describe the novel design of the positron extraction from the Surko trap and of the bunching system 2) show the advance in the construction of the set-up, presenting a systematic characterization (energy spread, positron yield, spin polarization) of the continuous positron beam produced by using three different solid rare gas moderators (Ne, Ar, Kr) [4] 3) illustrate the first planned experiment to measure the entanglement of the three annihilation gammas of ortho-positronium prepared into vacuum in selected quantum states.

[1] **Forward emission of positronium from nanochanneled silicon membranes**
S. Mariazzi , B. Rienäcker, R. Magrin Maffei , L. Povolo , S. Sharma, R. Caravita , L. Penasa , P. Bettotti, M. Doser, and R. S. Brusa
PHYSICAL REVIEW B **105**, 115422 (2022)

[2] **Classical modeling of positronium cooling in silicon nanochannel plates**
Francesco Guatieri , Sebastiano Mariazzi, Christoph Hugenschmidt, and Roberto S. Brusa
PHYSICAL REVIEW B **106**, 035418 (2022)

[3] **Design of a bunched positron beam extracted non-adiabatically from a Buffer-Gas Trap and focused in a free field region**
L. Povolo, S. Mariazzi, L. Penasa, R. Caravita, and R. S. Brusa
PHYSICAL REVIEW ACCELERATOR AND BEAMS: in print (2023)

[4] **Systematic characterization of Ne, Ar, Kr solid rare gas moderators and measurement of the spin polarization**. In preparatio (2023)

An Intense Spin Polarized Cold Positron Beam in a Magnetic Field-Free Environment

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We have constructed a pulsed positron beam system that produces dense spin-polarized positron bursts containing $1x10^7$ positrons in 25 μm FWHM and 5 ns FWHM, equivalent to an instantaneous current density exceeding 10 A cm^{-2}. The system utilizes a Na^{22} source and makes use of many technologies starting with a solid rare gas moderator [1] followed by a Surko style Penning-Malmberg trap [2,3] producing pulses of about $4x10^5$ positrons at a rate of 2 Hz. The pulses are transported by a bent 250 G solenoid over a 10 m path to a UHV positron accumulator [4] in a uniform magnetic field of 600 G, where the positrons are compressed using the rotating wall method at 80 MHz [5,6]. 5 ns pulses containing 5×10^7 positrons are produced at a rate of one per 75 s by a buncher-accelerator with abrupt magnetic-field termination [7,8]. The pulses are focused onto a thin Ni (100) foil remoderator which increases the brightness [9] and produces a 1.1 eV [10] polarized positron beam of $1x10^7$ positrons in a magnetic field free environment. The positrons are accelerated and focused onto a target in a spot about 25 μm FWHM in diameter and with a 5 ns FWHM. We measure the positron spin polarization to be (30.2±0.4) %. This system is uniquely suitable for production and spectroscopy of exotic matter-antimatter molecules such as the di-positronium molecule and the positronium-plus ion. With some modifications and improvements our system may yield sufficiently high current densities for the production of a neutral positron-electron plasma as well as a positronium Bose-Einstein Condensate [11].

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Development of the new low-energy-positron-diffraction (LEPD) experimental station at the Slow Positron Facility in KEK

R. Ahmed[a], I. Mochizuki[a], K. Ozawa[a], S. Mizuno[a], T. Hyodo[a], K. Wada[a]

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The crystalline surfaces have interesting features that differ from the bulk but are often so complex that they are difficult to reveal by conventional measurement and analysis. Low-energy positron diffraction (LEPD), the positron counterpart of the low-energy electron diffraction (LEED), is predicted to be an ideal method for studying surface atomic arrangements [1]. An LEPD system using a linear accelerator-based slow-positron beam was developed at the Slow Positron Facility of the Institute of Materials Structure Science, KEK [2]. We report on a major upgrade of the LEPD experimental station for the precise analysis of surface atomic arrangements.

We have developed an accurate and reproducible sample manipulator to adjust the sample position and orientation to achieve normal incidence of the beam on the sample surface. We have also developed a new sample holder that can be cooled by liquid nitrogen within very short period of time. This is necessary because LEPD, like LEED, is sensitive to the Debye-Waller factor. A dedicated sample preparation chamber is used for current heating, Ar^+ sputtering, deposition of various atoms and gas introduction. The prepared sample surfaces can be checked by a conventional LEED/AES spectrometer. The prepared sample holder is transported to the adjacent LEPD measurement chamber in UHV using transfer rod.

We have observed LEPD patterns for Cu(001) with the new LEPD station from 40 eV to 352 eV in 2 eV steps for 5 minutes each before surface contamination. The measurement time is now nearly two orders of magnitude faster than that in the initial data acquisition. Samples prepared at the LEPD station were also transported in a UHV transfer vessel to the IMSS Photon Factory, and angle-resolved photoemission spectroscopy (ARPES) observations were performed to investigate the surface electronic states.

Reference

[1] S. Y. Tong, surface science 457, L432 (2000).
[2] K. Wada et al., e-J. Surf. Sci. Nanotech. 16, 313 (2018).

Formation of a micrometer positron beam at the Scanning Positron Microscope

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To investigate inhomogeneous 3D-defect distributions on the micro-meter scale, e.g. close to fatigue cracks or dispersive alloy, with positron annihilation lifetime spectroscopy a monochromatic pulsed positron beam of variable energy with a diameter in the range of 1 µm and a pulse width of 150 ps FWHM is needed.

To this aim the Scanning Positron Microscope (SPM) was developed and built at the Universität der Bundeswehr [1]. To overcome the limit of low count-rates and corresponding exceedingly long measurement times the SPM is transferred to the intense positron source NEPOMUC at the MLZ in Garching. To connect the SPM to NEPOMUC a special interface has been constructed.

A sophisticated beam preparation, including multiple remoderation steps, is needed to reach a lateral resolution in the micro-meter range. An essential component of the interface is the positron elevator which compensates for the energy loss caused by the remoderation process without altering other important beam properties like time structure and brightness [2]. This device allows also keeping both, the source and the sample, at the same electrical potential.

During the long reactor shut down at the MLZ the SPM has undergoes a complete overhaul. The installation of the SPM is now complete and it is ready for first test measurements. We will present technical details of the SPM interface, the positron elevator and the SPM.

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C. Na-22 Source based experiments in volume

Tribolayer defect profiling using conventional positron lifetime technique

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Positron annihilation spectroscopy can be very useful in studies of tribological problems.

It has been well documented that near the surface exposed to the sliding a tribolayer with refinement grains is generated. Its thickness is a few micrometers and can be detected using the conventional positron annihilation techniques [1, 2]. The technique of sequential etching of a sample and measurements of the positron lifetime spectrum or the annihilation line shape parameter allows for the detection of open volume defects that occur in this layer and additionally their depth distribution. The measured annihilation characteristics, however, result from the entanglement of the positron implantation profile and the actual value of these characteristics at different depths. To get the latter, you need to invert the experimental results.

Two approaches to this inversion procedure will be presented during the lecture. Their application will be demonstrated on several experimental examples of the tribolayer obtained in Sterling silver, pure copper, and vanadium. These considerations will also be preceded by a discussion on the positron implantation profile.

The presented methods are applicable to the testing of the damage layer arising during many technological processes such as cutting, rolling, shot blasting and others used in industry. This extends the use of the positron annihilation technique to new applications.

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Positronium chemistry of a $Fe^{2+/3+}$ solution under electrochemical control

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Recently we have demonstrated with the $Fe(CN)_6^{3-/4-}$ redox couple that electrochemical processes in aqueous electrolytes can be monitored by positron and positronium annihilation [1]. This contribution will address the advantages of such measurements for studying the more application relevant $Fe^{2+/3+}$ system [2]. For this novel approach to positronium electrochemistry, a suitable cell setup is used, which allows simultaneously both electrochemical measurements and positron annihilation spectroscopy. Due to the different positronium chemistry of Fe^{2+} (spin conversion) and Fe^{3+} (total positronium inhibition and oxidation), the $Fe^{2+} \leftrightarrow Fe^{3+} + e^-$ redox reaction can be tracked *in situ* by means of positron lifetime measurements upon slow cycling voltammetry or galvanostatic charging. The variation of the mean positron lifetime with the $Fe^{2+/3+}$ concentration ratio could be quantitatively described by a reaction rate model for positronium formation and annihilation. An asymmetric change in the mean positron lifetime with applied potential, as compared to the simultaneously recorded symmetric current–potential curve, shows the stronger influence of Fe^{3+} on the characteristics of positronium formation and annihilation, as compared to Fe^{2+}. The highly reversible galvanostatic charging behavior monitored by positron lifetime underlines the attractive application potentials of positronium electrochemistry for *in situ* studies of iron-based redox-flow battery electrolytes.

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[2] P. Brunner et al., J. Chem. Phys. **157**, 234202 (2022)

Vacancies in Prussian White Cathode Materials employing Positron Annihilation Spectroscopy

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We are presenting a novel attempt to characterise Prussian blue analogues. Prussian White samples have been synthesised with different sodium content and then, characterised by common methods (ICP-OES, TG, SEM) but also by Mösbauer spectroscopy. We prepared three different sample states: fully and half-sodiated as well as de-sodiated. As a new method positron annihilation lifetime spectroscopy (PALS) has been applied to characterise the different samples states. We can state that the method of PALS gives reasonable results for Prussian White with varying sodium and water content. The relative intensity of the longer positron lifetime component (405ps) is increasing with deceasing sodium content, which is an indication that the positron "sees" less of the open crystal channels filled by movable ions, since those become more and more occupied by intercalated Na-atoms. This first attempt aims to present the potential of PALS to characterise Prussian Blue analogue materials with respect to defects and occupation of its crystal channels by movable ions.

Investigation of defects production using positron life time measurement and its effect on the nano-hardness under 120 MeV Au^{+7} ion irradiation in NiCoCrFePd High Entropy Alloy

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Single phase NiCoCrFePd high entropy alloy (HEA) are known to be radiation damage stable due to its distorted structure [1-2]. Thus, bulk samples of NiCoCrFePd HEA synthesized using arc melting method are irradiated with 120 MeV Au^{+7} ions at different ion fluence. X-ray diffraction (XRD) of pristine and irradiated samples show that the single phase remains stable up to the highest fluence of 1×10^{14} ions/cm^2. The value of life time components τ_1 = 151.9 ± 0.20 ps and τ_2 = 284.8 ± 0.7 ps are evaluated from the positron annihilation life time spectroscopy (PALS) measurement show presence of vacancy defects in the pristine sample itself. However, at initial ion fluence (3.3×10^{12} ions/cm^2) the value of τ_1 increases to 158.0 ± 0.4 ps along with the reduction in the intensity indicates the formation of dislocation defects and in the subsequent ion fluence the observation of slight decrease in τ_1 to 155.1 ± 0.4 ps and huge reduction in the intensity indicates further increase in the dislocation density. At the highest ion fluence 1×10^{14} ions/cm^2 huge increase in I_2 along with reduction in I_1 and with value of τ_2 = 258.0 ± 00.4 ps indicates the formation of vacancy clusters which is in consistant with the XRD analysis. The nano-indentation hardness show that the harness increases from 2.791 ± 0.624 GPa to 2.839 ± 0.406 GPa on the irradiation at initial ion fluence. Huge increase in the hardness was observed till ion fluence 3.3×10^{13} ions/cm^2 due to further production of dislocation defects, however at the highest fluence (1×10^{14} ions/cm^2) the reduction in hardness to 4.821 ± 0.602 GPa was observed from a value of 5.024 ± 0.424 GPa due to the collapse of vacancies/dislocation into cluster defects.

References:

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18-18 Jul 2023

D1 . Positron Confinement in Vacuum

Towards a low energy electron-positron plasma in the lab

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Positively and negatively charged particles with equal mass can form a pair plasma. For example, this can occur in extreme astrophysical environments that generate electron-positron pairs at sufficient density for collective effects to emerge. The mass symmetry distinguishes pair plasma from the more familiar ion-electron plasma, and many conventional instabilities are thought to be suppressed. The APEX collaboration aims to verify this by creating a low-energy positron-electron plasma in the lab. The experiments will require an unprecedentedly large collection of low-energy positrons. I will present the current status of the APEX project, including the development of a buffer-gas trap for the high-intensity NEPOMUC beam and the results of preparatory work regarding the injection of positrons into a nonneutral electron plasma. In addition, I will review the latest progress in the design, construction, and diagnostic development of a levitated dipole trap and a compact optimized stellarator (EPOS). These two devices will be used to magnetically confine an electron-positron plasma, allowing this intriguing substance to be studied---for the first time---at low energy and over long timescales.

Fast Toroidal and Slow Radial Expansion of Positrons in a Magnetic Dipole Trap

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We present the first injection and confinement of positron pulses in a magnetic dipole trap, along with novel measurements of the dynamics of these processes using an array of 25 gamma detectors. A buffer-gas trap (BGT) accumulates positrons generated by the AIST Linac source [1] and extracts them as a 6 eV pulse. Electrostatic potentials applied to electrodes at the edge of the dipole field induce cross-field transport through ExB drifts, to inject positrons [2]. Efficient injection is characterized by a strong delayed annihilation signal in the absence of a prompt signal on Bismuth-Germanate (BGO) detectors configured for pile-up measurements. The delayed signal indicates annihilation due to re-encountering the injection potential after an almost completed toroidal orbit whereas a prompt signal indicates losses during injection. A movable probe allows for radial profile measurements.

Switching the injection electrode potentials off before the positrons have completed a toroidal rotation results in confinement [3]. The early confinement is characterized with (partial) dumps of the non-mirror trapped positrons onto the central magnet by switching off its positive bias and (full) dumps of all remaining positrons onto the walls by reapplying the injection potential. The resulting pile-up annihilation signals detected at three toroidal angles characterize the expansion of the positrons within the first few hundred microseconds.

Additional measurements were performed using long hold times (>1s) and 22 toroidally distributed BGO detectors calibrated for 511 keV photons. In this case, annihilation events were detected individually as they occurred. The nanosecond timing resolution and large solid-angle coverage were exploited to locate sources of annihilation with coincident lines of response and the distance-dependent signal fraction on each detector.

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The APEX collaboration receives/has received support from IPP/MPG; the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme; the Helmholtz Association; the Deutsche Forschungsgemeinschaft (DFG); the Alexander von Humboldt Foundation, the Helmholtz Postdoc Programme; the UC San Diego Foundation; the United States Department of Energy, the Japan Society for the Promotion of Science (JSPS); and the National Institute for Fusion Science (NIFS).

D2. Anti-Hydrogen Experiments

Recent advancements at AEgIS for efficient pulsed antihydrogen formation

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Antimatter research has been exploring the potential applications of positrons and positronium in a wide range of fields, from materials science to fundamental studies. At the AEgIS (Antimatter Experiment: gravity, Interferometry, Spectroscopy) collaboration at CERN, recent developments have been made in the efficient formation of antihydrogen using the charge exchange reaction between Rydberg-positronium and cold trapped antiprotons. One of the major advancements is the implementation of a fully automated control system that has been adapted for the 24/7 pulsed antiproton beam from the ELENA (Extra Low ENergy Antiprotons) decelerator. This system has led to improved efficiency and consistency in the experiment. Another crucial development is the use of morphologically tuned nano-structured silicon targets, which have proven highly efficient in converting positrons to positronium, with a significant fraction of the emitted Ps cloud being thermal.

The experimental scheme has also been improved to generate more positronium and higher Ps Rydberg levels with a double-pass laser, as well as to trap more and colder antiprotons in an optimized low-noise Penning-Malmberg trap. In fact, a record-breaking 3.7 million antiprotons in a single shot from ELENA with kinetic energies below 14 keV were trapped in 2022, enabling the production of a high-intensity pulsed antihydrogen source [1]. This breakthrough will be crucial for future precision measurements of the gravitational acceleration of antimatter.

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Positron manipulation and control at the ASACUSA Cusp experiment

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The ASACUSA-Cusp experiment aims to perform spectroscopy of the hyperfine structure of antihydrogen by producing a beam of cold, spin polarised, ground state antihydrogen. The beam will be produced by mixing positrons and antiprotons in our unique Cusp trap which uses a pair of superconducting coils in an anti-Helmholtz configuration to produce a magnetic field capable of both confining the charged particles radially and polarizing the antihydrogen atoms.

Thus far, the collaboration has observed antihydrogen 2.7 m from the production region [1] and measured the distribution of principal quantum number of these atoms [2]. This weak beam was not suitable for the spectroscopy measurement so work commenced on improving the beam intensity and skewing the distribution towards ground state atoms. Simulations showed that the route towards this aim was producing colder dense positron plasmas [3].

Recently, a major technological milestone was achieved by the collaboration. Antihydrogen produced via three-body recombination will have an isotropic distribution so a large open solid angle is needed for the antiatoms to escape. This has the disadvantage that the production region is illuminated by a hot (300 K) black body. Previously, it has not been possible to cool plasma below 130 K, however, a new electrode stack and coldbore with a focus on blocking microwaves from the room temperature region has allowed particles to cool to 25 K maintaining the large open solid angle for the beam to escape [4].

In this presentation I will discuss the methods used by the ASACUSA Cusp experiment to manipulate and control positrons and give details on the most recent work on plasma handling and beam production in the new Cusp trap.

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Antihydrogen production for the GBAR antimatter gravitation experiment

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The weak equivalence principle is a cornerstone of Einstein's general theory of relativity. Its validity for antimatter has never been directly tested. The GBAR (Gravitational Behaviour of Antimatter at Rest) experiment aims to do this by measuring the free fall of the simplest antimatter atom, antihydrogen, in the Earth's gravitational field. The experiment requires antiatoms at extremely low temperatures, on the order of 10 µK. Since it is not possible to cool neutral particles down to this temperature range, GBAR proposes to first create positively charged antihydrogen ions made up of an antiproton and two positrons. These ions can then be cooled to the extremely low energy using laser-cooled beryllium ions. After removing the excess positron by photodetachment, the time of free fall can be determined. The experimental apparatus has been installed at CERN's ELENA decelerator ring, which provides antiprotons with a kinetic energy of 100 keV. The antiprotons are then further decelerated to 6 keV by a switched drift tube in the GBAR beamline. The positrons are produced by a 9 MeV electron linac, trapped in a buffer gas trap and collected in a 5 T high field Penning-Malmberg trap. The anti-ions are created in two consecutive reactions in a positronium target cloud.

GBAR has reached an important milestone with the detection of the first antihydrogen atoms formed by 6 keV antiprotons in a positronium cloud in a charge exchange reaction in 2022. We present the experimental setup and the results of the detection of the first anti-atoms.

D3. Positronium Atomic Physics

Production of a metastable 2^3S_1 positronium beam

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Energy tunable positronium beams generated from the charge-exchange of positrons with atomic and molecular gases held in a cell have been used for many years to investigate positronium production (e.g. [1]) and its interaction with matter (e.g. [2]). Murtagh *et al.* [3] showed that approximately 26% of positronium atoms produced from positron collisions with xenon are in the 2P state. This result implies that an energy tunable beam of metastable 2^3S_1 positronium atoms can be realised in a similar way.

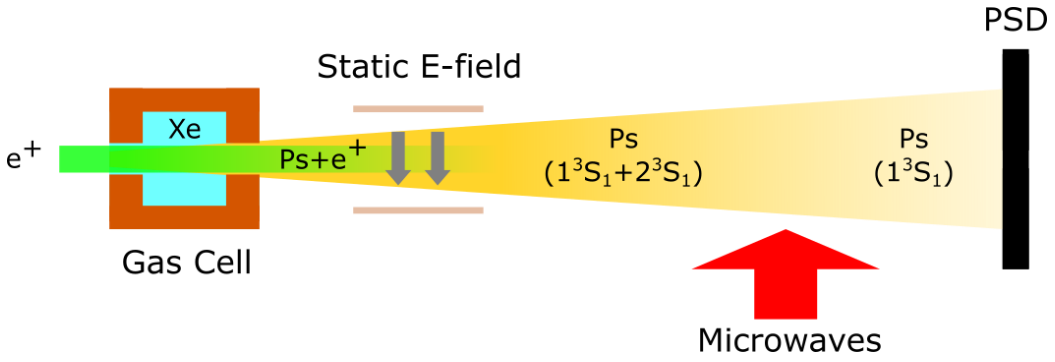

Figure 1: *Schematic of the experimental arrangement used in the production and detection of the 2^3S_1 positronium beam.*

Here, the production of such a beam is demonstrated using the experimental arrangement shown in figure 1. Microwave radiation is used to drive the 2^3S_1 component of the positronium beam to the ground-state via the intermediate 2^3P_2 state (fluorescence lifetime 3.1 ns). The beam divergence is determined directly using a position sensitive detector. The 2^3S_1 beam may be used for performing fixed or frequency offset Ramsey separated oscillatory field measurements [4].

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Positronium manipulation with long laser pulses

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We report on the development of an experiment designed to demonstrate positronium (Ps) laser cooling. The apparatus entails a positron beamline, a 100 ns laser pulse driving the $1^3S \rightarrow 2^3P$ transition for Doppler cooling and a 3 ns laser pulse driving the $1^3S \rightarrow 3^3P$ transition for Doppler velocimetry by two photon resonant ionization [1]. Ps is produced by implantation of positrons in a nanochannel target in a magnetic field free environment. Both single shot positron annihilation lifetime and photo-positron imaging on a micro channel plate [2] are used to perform spectroscopy on Ps.

Instead of quenching, we observe an increase in the Ps annihilation lifetime by excitation in the 2^3P state confirming the absence of magnetic field in the Ps production area and a long Ps-laser interaction time. In order to enhance control over the end of the Ps-laser interaction time, a fast opto-electronic switch is implemented inside the laser oscillator to induce a sharp falling edge in the laser pulse profile with a few nanoseconds' precision. In this way, it is possible to ensure that most of the atoms have relaxed to the ground state when probing the velocity distribution on the $1^3S \rightarrow 3^3P$ transition.

The most recent results obtained with this setup will be reported.

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Precision spectroscopy of the positronium *n* = 2 fine structure

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Positronium (Ps) is a purely leptonic system making it a useful testbed of quantum electrodynamics. The Ps $n = 2$ fine structure intervals are some of the most precisely calculated transitions in Ps at an uncertainty of 7 ppb [1]. This makes them a good target for experimental measurements, but recent studies have revealed shifts and asymmetries in the transition line shapes [2] which have been explained by reflection effects of the microwave field causing frequency dependent power variation across the line shape [3].

We have used free-space microwave radiation to explore this rf reflection effect, confirming the large shifts this effect can induce on broad line shapes without causing significant asymmetry. We have performed the best precision measurement to date on the $2^3S_1 \rightarrow 2^3P_2$ interval using a modified waveguide technique, designing an experiment to minimise reflection effects and obtaining a value of 8627.87 ± 0.34 MHz, which is 3.4 standard deviations higher than the theoretical value of 8626.71 ± 0.08 MHz.

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Modelling Positron Transport in the Positronium Formation Regime

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In positron annihilation studies, positrons are produced with a broad energy distribution well above thermal energies. They thermalize through collisions with the gas, before eventually annihilating. For energies between the positronium formation threshold (~5.3 eV in Xe) and the ionization threshold (~12.1 eV in Xe) a significant fraction of the positrons form positronium.

To study this nonequilibrium process, a time-dependent, multi-term, Boltzmann-equation solver has been developed for positron transport [1,2]. In the low-energy regime below the ionization threshold energy, cross-sections for the electronic excitation, positronium formation, differential elastic scattering and annihilation are the most important inputs from which transport properties including the average annihilation rate can be calculated. The transport of para-positronium and ortho-positronium are subsequently modelled using rate equations, with pick-off annihilation effects incorporated into the latter.

Here we will discuss our investigation of how each scattering process influences transport properties in gaseous xenon, with a particular emphasis on the average Zeff, which are compared to experimental measurements [3]. Additionally, we will discuss generalizing these results to other noble gases and comment on the application to other physical systems [4].

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E. Data Analysis tools

New Evaluation Software for Coincident Doppler Broadening Spectroscopy

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Coincident Doppler Broadening Spectroscopy (CDBS) enables the non-destructive investigation of open volume defects such as vacancies and their chemical environment. In addition, precipitates with higher positron affinity than the host matrix can also be analyzed, giving insights into precipitation processes in structural materials. The CDB Spectrometer at the Neutron induced Positron Source Munich (NEPOMUC) has recently been upgraded and now features ten High Purity Germanium (HPGe) detectors, significantly decreasing the measurement times at the instrument. To handle the increased data output of the instrument a new data analysis software package was developed named Software Tools for Analyzing CDB Spectra (STACS) [1]. STACS can efficiently handle the large 2D arrays generated by CDBS. It can visualize CDBS data and includes a wide range of tools to analyze CDB spectra for further evaluation. In this contribution the main analysis function of STACS, i.e., the extraction of the Doppler broadened positron-electron annihilation line from 2D CDBS histograms will be demonstrated. Additionally, several other features will be shown including the generation of ratio curves using measurements on age-hardened AlCu alloys, as well as, the analysis of high statistics measurements performed on W and Kapton.

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Analysing toolkit for positron annihilation spectroscopy experiments

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In positron annihilation spectroscopy (PAS) experiments, the determination of the fraction of positrons annihilating inside each layer of a multi-layer configuration is of the primary concern of PAS experimentalists. Knowledge of the annihilation intensity in each layer of a multi-layer configuration of different materials plays an essential role in analysing a measured positron lifetime spectrum for evaluating the individual lifetime components using computer-based deconvolution algorithms [1]. Positrons traversing an absorber material exhibit a property of implantation profile over the penetration depth [2]. Generally, the profile behaviour depends on the positron energy characteristics, linear absorption coefficient α^+ of the implanted material [3], the type and thickness of the supporting foil (when using a radioactive source), and the backscattering processes at interfaces between adjacent layers of different materials in the case of a multi-layer measurement configuration. Moreover, the source contribution (SC) associated with the fraction of positrons annihilating in the β^+ source and the supporting foil is crucial in obtaining an accurate PAS spectral analysis [4]. However, there is not a complete theory available addressing the complex energy fading and multi-scattering processes undergone by positrons penetrating the multi-layer configuration yet.

Based on theoretical and experimental investigations, the aim of our research is to establish a practical toolkit for PAS experimentalists to obtain an accurate implantation profile estimation and positron lifetime spectral analysis. This toolkit is featured by comprehensive functionality, high analytical accuracy, versatility and universality, and an utmost user-friendliness with a designed user interface.

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LIMPID – A New Analysis Tool for Variable Energy Doppler-Broadening Spectroscopy Applied to Multilayer Systems

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We developed a new analysis tool for positron depth profiles recorded by variable energy Doppler-broadening spectroscopy, called LIMPID (Layer-wise Investigation of Measurements on Positron Implantation and Diffusion). It allows the extraction of positron diffusion lengths by fitting the measured lineshape parameters of the 511 keV annihilation photo peak as a function of implantation energy. The code is written in Python and open source, thereby easily accessible and adaptable. In this talk we present the theoretical background of the algorithm implemented, which includes a solution of the time-independent positron diffusion equation. By taking into account sample properties such as mass density, composition and positron affinity, apart from the positron diffusion length LIMPID can also be used to determine sample parameters like, e.g., layer thicknesses in multilayer systems. We demonstrate the main features of LIMPID using recently recorded data obtained from Cu/Cr bilayers on a Si substrate. Furthermore we discuss the performance of the new analysis software and compare it to VEPFIT [1], the currently most popular tool for depth resolved DBS.

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Posters I

Vacancy-Type Defects Just below Fracture Surface by Positron Probe Microanalyzer

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Fracture in plastic deformation of metals is caused by localized stress accumulation, which is expected to lead to a formation of a lot of vacancies. On the other hand, detection of defects just below the fracture surface is necessary to elucidate the mechanism of the fracture, but it has not been achieved yet. In this study, we aimed to measure the vacancies just below the fracture surface of metals, pure Ni, using positrons. The positron probe microanalyzer (PPMA)[1], in which a positron microprobe can be injected with a diameter of 100 μm into the vicinity, or a few hundred nm, of a surface is suitable for the defect analysis on a fracture surface.

The PPMA installed at AIST uses a linac-based highly-intensive positron source and enables positron lifetime measurement by converting a pulsed positron beam. The beam diameter was about 150 μm, the injection energy was 8 keV (average injection depth 550 nm), the counting rate was about 50 cps, and the time resolution was 240 ps. The sample was pure Ni (99 %). It showed an intragranular fracture in normal strain (fractured at 56 % strain), while it showed an intergranular fracture (fractured at 34 % strain) in straining in hydrogen environment.

In the gauge region of the normally fractured sample, a dislocation component of 169 ps and a long-lifetime component of 360 ps were measured by PPMA. Since only the dislocation component was detected in the bulk analysis, the long-lifetime component was attributed to the Ni oxide film on the surface. On the intragranular fracture surface, two components, 179 ps and 400 ps, were detected by PPMA. The long-lifetime component was attributed to a vacancy cluster because it was longer than that for the Ni oxide film. These results indicated that a lot of vacancies were induced by localized dislocation accumulation below the fracture surface and stabilized by forming vacancy clusters, although monovacancies are unstable at RT.

Much longer component of 444 ps as well as 189 ps due to dislocation was measured at the grain boundary fracture surface in hydrogen embrittled Ni by PPMA. A 444 ps component was considerably longer than the lifetime of 317 ps measured in the bulk analysis, indicating that vacancies were densely formed just below the grain boundary and they are transformed into larger vacancy clusters.

This is the first measurement of vacancies just below the fracture surface of a metal and we will apply PPMA to investigate the role of vacancies in a mechanism of fracture in various metals.

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Multicomponent Quantum Mechanics/Molecular Mechanics Study of Hydrated Positronium

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Positrons and positronium (Ps) atoms have long been known as nanoscale probes in materials sciences. Positron Annihilation Lifetime Spectroscopy (PALS) measurements has been applied to investigate conformational, structural, and microenvironmental properties of biomimetic systems [1], as well as phase transitions of lipid bilayers [2] and pharmaceutically relevant compounds [3]. The Ps contribution to the annihilation signals is expected to allow improvement of accuracy and diagnosis in Positron Emission Tomography (PET) as indicated in recent studies [4,5]. Motivated by the biomedical applications mentioned, we have combined computational techniques to model Ps atoms in water. We considered the sequential Quantum Mechanics/Molecular Mechanics (s-QM/MM) approach [6], composed by classical simulations (MM step) followed by quantum calculations (QM step). The MM step consider a force field composed by the Lennard-Jones potential to describe Ps-solvent interaction during classical Monte Carlo (MC) simulations, this step provides liquid structures and the thermodynamical properties indicating a hydrophobic character of Ps. The QM step consider the Ps-solvent configurations for quantum calculations with the Any Particle Molecular Orbital (APMO) method [7], which generalizes the electronic structure techniques for systems with more than a single fermionic species. The Hartree-Fock wavefunctions obtained were considered to account the pick-off annihilation rates and vertical detachment energies of hydrated Ps. Our results were recently published [8] indicating a promise protocol to simulate the solvated Ps, that can be extended to more complex systems in liquid phase.

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Characterization of proton irradiation induced defects in metals: complementarity of positron annihilation spectroscopy and resistivity Recovery.

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Materials in nuclear reactors, such as austenitic steels, are subjected to harsh operation conditions: temperature, pressure and irradiation. Irradiations by high-energy particles, induce significant changes in their properties on both macroscopic and microscopic scales. Thus, their performance and lifetime can be strongly impacted and understanding of the evolution of materials under irradiation is of major importance. Our project focuses specifically on the determination of the distribution of primary defects (their nature and proportions) after ion irradiation. In this framework, different experimental complementary techniques are used such as the Resistivity Recovery (RR) and the Positron Annihilation Spectroscopy (PAS). Each technique is sensitive to different types of defects and their combination should provide a better knowledge of the damage induced in metals. In this study we focus on pure metals and model alloys (Fe, Ni, NiCr…).

A device for measuring resistivity as a function of sample temperature (from 40 to 300 K) has been developed at CEMHTI. The methodology for sample preparation and mounting as well as the precise measurement of resistivity have been optimized. This device can be installed on one of the beam lines of the Pelletron ion accelerator and allows in situ measurements under low temperature irradiation.
First, the resistivity of 99,99% pure iron foil was measured as a function of temperature before irradiation. Low temperature 2.8 MeV H+ irradiation (49 K) was performed and the evolution of the resistivity at low temperature was measured as a function of annealing temperature over the range from 50 to RT in order to record the resistivity recovery (RR) in thin iron sheets. Irradiation induced an increase in resistivity (measured at 49K) which is comparable to that obtained in the literature. After irradiation, RR measurements showed a decrease of resistivity due to the increase of defects recombination. The annealing stages are extracted and can be associated with different type of defect by comparison with literature. The sample is then characterized using slow positron beam coupled with a Doppler broadening spectrometer after annealing at RT. The PAS and RR results are compared to identify the vacancy distribution still in the sample after irradiation and annealing at 300K.

Can point defect density explain the critical current degradation and recovery in cryogenically irradiated and annealed high-temperature superconductors?

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Superconducting magnets made of yttrium barium copper oxides (YBCO) can carry large currents in high magnetic fields. This property is known as the critical current and enables compact fusion designs such as the ARC reactor. But the critical current, J_c, degrades under the bombardment of fast neutrons born in the deuterium-tritium reaction. To study the radiation tolerance of YBCO in a fusion environment, we developed a cryogenic irradiation facility where J_c can be measured before, during and after irradiation. We observe a few percent increase in J_c at low dose, followed by a monotonic decrease at high fluences. Our results also show that J_c recovers by up to 20% of its initial value when the sample is warmed up to 300 K. Altogether, these observations suggest an important role of smallest defects, which can cluster or annihilate well-below room temperature. In principle, measurements of vacancy and void concentrations using a slow-positron beam lifetime spectroscopy could clarify the microstructural origin of the critical current degradation and recovery. This technique is effectively non-perturbing, and compatible with thin film single crystal samples, which closely resemble the coated conductors used to wind YBCO magnets. However, quantifying vacancies in a complex oxide can be challenging due to the variety of possible defects and the inherent difficulty of procuring defect-free samples, both needed to constrain the bulk and vacancy lifetimes. We present initial work on DFT simulations of positron lifetimes in YBCO, and experimental considerations to measure the critical current and the concentration of radiation-induced defects in parallel. Developing a mechanistic understanding of critical current degradation is key to minimize the neutron-shield thickness, and optimize the overall size and cost of fusion reactors.

Effects of an external electric field on the ortho-positronium lifetime in a silicon-dioxide thin-layer

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The interface between two different materials is of great concern in optimizing electronic or optoelectronic properties of layered semiconductor systems, because at the interfaces additional defects can occur, e.g. due to the lattice mismatch of both materials. The energy and material-density dependent depth-distribution of monochromatic, low-energy positrons implanted and thermalized in condensed matter makes the investigation of interfaces virtually impossible. From the positron diffusion trapping model it is well known, that an electric field, intrinsic or extrinsic, can alter the diffusion behaviour of thermalized positrons [1, 2]. Therefore, by applying an electrical field, positrons may be drifted towards the interface or away from it.
This was experimentally shown by doppler broadening spectroscopy on Au/Si Schottky diods [3] and on Metal-Oxide-Semiconductors [4, 5]. However, this kind of experiments are yet to be reported with positron-annihilation lifetime spectroscopy. Here, we present our first measurements with external bias up to 6.5MV/cm applied to a 180nm silicon oxide layer with a 50nm Aluminum gate conducted at the MePS instrument.

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Investigation of microstructure of multi-principal element thin films (Ti-Zr-Nb-Hf-Ta) with binary, ternary, and quaternary composition

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High-entropy alloys (HEAs) are a new concept in materials science due to their complex composition of typically principal 5 elements of high concentrations. HEAs exhibit unique physical properties, e.g. mechanical properties, hydrogen absorption capacity, or irradiation resistance. The high configurational entropy of random solid solution (SS) significantly reduces Gibbs free energy, which stabilizes the random SS at the expense of the mixture of ordered intermetallic phases, particularly at high temperatures. Local distortions of a crystal lattice are a typical feature of HEAs and are caused by different atomic sizes of elements. Local variations of lattice parameter can be expressed by the empirical misfit parameter δ, defined by atomic radii and concentrations of constituting elements.

The preparation of HEAs in a form of thin films provides an excellent opportunity to study various microstructures, which cannot be easily achieved in a bulk form. In the presented study, the microstructure of thin films prepared by magnetron sputtering with the composition derived from the Ti-Zr-Nb-Hf-Ta system was investigated by XRD, SEM, and positron annihilation lifetime spectroscopy. Films characterized by small misfit parameter δ (binary NbTa and HfZr, ternary NbTaTi and HfTiZr) exhibited nanocrystalline structure. For the films with the composition characterized by large misfit parameter δ (binary NbZr, ternary NbTiZr, quaternary HfNbTaTi and HfNbTaZr) the deposition at room temperature resulted in an amorphous structure. Both small-δ and large-δ films exhibited nanocrystalline structure when the deposition temperature was increased to 600°C. Positron annihilation lifetime spectroscopy was carried out on the pulsed positron beam facility MePS. On the atomic scale, amorphous films are characterized by a relatively open structure with a high concentration of vacancy-like defects and also large vacancy clusters, unlike the more compact nanocrystalline films, where vacancies associated with grain boundaries were the dominant type of defect.

Conceptual design of a slow positron beamline using a 30 MeV L-band LINAC

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Energy-variable monoenergetic positron beams (slow positron beams) have been effectively used to investigate vacancy-type defects in thin films or near-surface layers of various functional materials. Slow positron beams are obtained from radioisotope-based positron sources but intense slow positron beams can be generated exclusively from large-scale experimental facilities such as nuclear reactors and accelerators. In terms of accelerator-based positron sources, so far, radiofrequency-driven electron linear accelerators (LINAC) have been extensively used. In principle, LINAC-generated positron beams are not continuous (i.e., pulse beams), while reactor-based positon beams are continuous. The pulse beams can be potentially applied for unique applications such as pump-probe type measurements [1].

A LINAC at Institute for Integrated Radiation and Nuclear Science, Kyoto University (KURNS-LINAC) has two acceleration tubes driven by L-band (1.3 GHz) radiofrequency. The KURNS-LINAC can generate 30 MeV electron beams with a repetition rate up to 100 Hz and a pulse width up to 4 μs. Higher electron beam intensities are expected for the L-band LINAC, compared with typical S-band (2.8 GHz) LINACs. Preliminary experiments using the KURNS-LINAC generated slow positron beams with intensities of $>10^7$ e^+/s [2]. But this beamline has been disassembled and it is not available. In this study, we aim to develop a new slow positron beamline and to use the beamline for in-situ and pump-probe type measurements.

A basic design of the beamline has been performed with a different arrangement from that of the previous study. By using the SIMION code for charged-particle trajectory simulation, the performance of the conventional beamline components such as mesh-shaped moderators, magnetically guided beam ducts and a linear storage section, have been evaluated for effective beam generation and transport. For example, the evaluation of the linear storage section indicated that the inaccurate alignment of guide coils leads to the spread of the stored positrons.

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Development of spin-polarized positronium time-of-flight method

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Using a spin-polarized slow positron beam, the electron spin polarization of top-surface layer can be determined because the positronium (Ps) is formed only at the vacuum side of metal surfaces [1, 2]. If an energy- and spin-resolved Ps annihilation spectroscopy is available, the density-of-states (DOS) of spin-polarized electron associated only with the top-surface layer will be obtained. This should be a powerful method to evaluate the spin polarization near the Fermi level, which is very important information for the development of the spintronics devices. We have developed the spin-polarized Ps time-of-flight (SP-PsTOF) apparatus in response to such offers [3].
A spin-polarized positron beam generated from a Na-22 source is transported to the sample by the electrostatic lenses. At low incident energy, Ps formed on the top of the sample surface ejects into the vacuum with the energies of several electron volts. This energy is determined using the Ps time-of-flight (Ps-TOF) method, which measures the time difference between the positron incident and ortho-Ps annihilation. From a difference of two Ps-TOF spectra obtained by alternating the magnetization direction of the sample, the energy-resolved spin-polarization of the surface electrons is obtained. Recently, we succeeded to improve both of Ps detection efficiency and time resolution by installation of a plate to prevent Ps from passing in front of the detector. We attempt to obtain the energy-resolved surface electron spin polarization of some spintronics materials, such as half-metals.

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Defects in aluminum rich Si-doped 90% AlGaN determined by positron annihilation and X-ray absorption spectroscopy

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We recorded Doppler broadening of positron annihilation radiation in Si-doped $Al_{0.90}Ga_{0.10}N$ layers grown by metal-organic vapor phase epitaxy on AlN/sapphire at room and elevated temperatures.[1] The Si doping was varied in the range from 9×10^{17} cm^{-3} to 1.2×10^{19} cm^{-3} at two growth conditions: a low V/III ratio of 200 at a reactor pressure of 50 mbar (series H) and for a high V/III ratio of 700 and a growth pressure of 200 mbar (series L).[2, 3] In series L, (high V/III ratio of 700 and a growth pressure of 200 mbar) we observe positron saturation trapping at cation vacancy defects present above 5.0×10^{18} cm^{-3} for all studied Si doping levels. We observe high V_{III} concentration probably due to low formation energy in these samples with low C content. Interestingly, when Si content approaches 10^{19} cm^{-3} PAS data shows a transition for the dominant positron trap from V_{III} to another defect, which we interpret as a high density of Si-DX centers.[4] In series H, the PAS results show the cation vacancy concentration increasing with the Si concentration from $<1\times10^{16}$ cm^{-3} to $>2.0\times10^{18}$ cm^{-3}. The reason for the lower V_{III} content is an order of magnitude higher level of C acceptors, which is shifting the Fermi level away from the conduction band edge and increasing the formation energy of V_{III}. In samples with three highest Si levels above 10^{19} cm^{-3}, negatively charged non-open volume defect appears with concentrations similar to the Si concentration as data points move closer to AlN lattice point similar to behaviour observed in L series with highest Si content. We further study the effect of local GaN- or AlN-like environments of Si atoms vs. Fermi level effect with help of x-ray absorption spectroscopy data.

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Open volume defects in ultra-thin TiO_2 layers embedded in VMCO-like samples

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Positron annihilation signals from VMCO-like samples, grown by atomic layer deposition at different temperatures are utilized for the characterization of differences in the open volume defects in the TiN/TiO_2/a-Si/TiN heterostructures [1]. The layer of interest had only a thickness of 15 nm and the total thickness of the sample structure was 43 nm. Doppler and coincidence Doppler mode of positron annihilation spectroscopy combined with a monoenergetic positron beam were used for this study. Differences observed in the Doppler parameters indicate differences in the positron trapping states of the TiO_2 epilayers grown at different temperatures. Furthermore, the coincidence-Doppler results show that these differences cannot be due to intermixing of the TiO_2 and a-Si layers and the formation of a thin SiO_2 layers at the interface during the growth process. The results indicate that the amount of open volume defects in the TiO_2 layer of the VMCO-structure seems to increase with an increase in the growth temperature.

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Monitoring the S-phase formation in a high-purity Al-Cu-Mg alloy by truncation during heating-up

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We are presenting a novel attempt to combine in-situ and ex-situ measurements for aluminium alloys. As a model alloy we have chosen an Al-1.7Cu-1.3Mg (at.%) alloy, which has been cast from high purity elements (5N5 Al, 4N Cu and 4N Mg). As basic method DSC (heating ramp: 5 K/min) has been employed to determine different states during S-phase formation: onset, maximum of the exothermal peak, end of exothermal reaction. Sample states were frozen-in by an abrupt truncation of the heating ramp (5 K/min), i.e. cooling quickly to room temperature. So, the current sample state is frozen-in. After truncation all samples have been measured without further preparation by X-ray diffraction (XRD) and positron annihilation lifetime spectroscopy (PALS). Thus, we could correlate exactly different sample states, which is impossible by conventional experiments, i.e. heating to a certain temperature and then holding a certain time. This paves the way to investigate defined and comparable sample states by methods, which require an extensive sample preparation, like TEM or 3DAP, and in-situ methods like DSC or XRD at synchrotron beam lines.

Defect Production and Positron Annihilation at Vacancies in Lead Iodide Perovskite Layers

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Hybrid organic-inorganic lead halide perovskites (HOIPs) attract much attention for their application in optoelectronic devices. However, the long-term stability remains one of the major concerns for the large-scale utilization of the perovskite technology [1,2]. Ion migration has been shown to be at origin of hysteresis in lead halide perovskites [3,4] and to play a dominant role at the interfaces [5]. This questions the existence and/or generation of defects in HOIPs and their role in defect-assisted mechanisms of ion migration under bias and light illumination near the interfaces.

This work focuses on vacancy-type defects. When in neutral or negatively charged states, such defects capture thermalized positrons in their open volume and give rise to annihilation fingerprints specific to the nature of the vacancy-type defects. Positrons have a most striking reproducible and stable behavior in $MAPbI_3$ layers spin-coated or CVD deposited on substrates. An intriguing property is the lack of response of the annihilation fingerprints to the production of defects in such layers after high energy implantation. The annihilation characteristics, e-_e+ annihilating pair momentum distribution, are consistent with annihilation fingerprints arising from capture at huge native vacancy concentration, $\geq 3*10^{18} cm^{-3}$, that efficiently capture thermalized positrons before their annihilation in pristine as well as irradiated layers. The nature of the dominant vacancies capturing positrons is discussed [6].

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F1. Defects in thin films (semiconductors, oxides..)

The Pulsed Low Energy Positron System PLEPS at the MLZ: present status, applications and future developments.

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The pulsed low energy positron system PLEPS [1] is a user facility at the intense positron source NEPOMUC at the MLZ in Garching, Germany [2] for defect depth-profiling with positron lifetime measurements.
PLEPS uses a monochromatic pulsed positron beam of variable implantation energy in a range between 0.5 keV and 22 keV and with 1 mm diameter. In situ manipulation of the sample is possible: The sample temperature can be varied between 80 K and 600 K. With a new tunable broad-band illumination system optically active defects can be detected and identified by manipulating their charge state. Positron drift experiments to explore interfaces and internal surfaces can be performed by applying bias voltages to the samples.
Typical applications of PLEPS comprise the defect identification in thin layers and layered structures of semiconductors [3] and insulators [4,5], the investigation of irradiation induced and other defects in materials for fusion and fission [6,7], as well as the characterization of open volumes in glasses, polymers and polymer- and membrane layers [8,9].
In this talk we will show the present setup of PLEPS together with some exemplary applications and discuss future developments.

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Vacancy defect identification in lead halide perovskites

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There is intensive focus on the development of metal halide perovskite solar cells are motivated by the unprecedentedly rapid increase in cell efficiency to values comparable to silicon. While this success has in been part attributed to defect tolerance and reports of modest defect densities [1]. Nevertheless, intense efforts are in progress to identify and quantify point defects in these materials [1,2]. Vacancy defects are a centrally important class hence positron annihilation spectroscopies are of directly relevance. The positron lifetime values are long in methylammonium (MA) lead iodide, $MAPbI_3$, and $MAPbBr_3$ due to the low electron densities [3,4], hampering deconvolution of different states. The lifetime ranges in these two model halide perovskites are different with $MAPbI_3$ exhibiting larger values. Device materials commonly involve compositions with mixed A-site and halide anions. For PAS to contribute it is first necessary to develop a clear understanding of positron trapping in the pure materials. In this work we report variable energy positron annihilation lifetime measurements were performed using the mono-energetic positron source beamline at Helmholtz–Zentrum Dresden–Rossendorf performed on a series of $MAPbBr_3$, $FAPbBr_3$ and $MAPbI_3$ samples and reported related TCDFT calculated positron lifetimes.

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Complementary insights into the photochromism of YH_xO_y thin films obtained by low energy positron and muon beam experiments

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Yttrium oxyhydride (YH_xO_y) is a promising mixed-anion semiconductor in view of its special photochromic properties, offering prospects for application in smart windows. The origin of the photochromism is topic of current investigations [1-3]. Here, we present complementary in-situ illumination studies based on positron annihilation spectroscopy (PAS) and muon spin rotation spectroscopy (MuSR). We will compare the experimental findings and techniques employed in the low energy positron and muon beam experiments, and discuss the insights gained into the photochromism.
Positron Doppler Broadening (DB-PAS) and Positron Annihilation Lifetime Spectroscopy (PALS) was applied to probe the evolution of the electronic structure and vacancies in YH_xO_y thin films [2]. The PALS studies reveal the presence of Y cation vacancies and nanopores in the as-deposited films. The reversible part of the changes in S and W parameters observed in the in-situ illumination DB-PAS studies suggests that the formation of metallic-like regions is a key ingredient in the photochromism. Low energy MuSR experiments on similar YH_xO_y thin films provide complementary insights into the nature of the photochromic effect and the role of hydrogen [3]. In-situ illumination leads to a reversible reduction in muonium fraction, most probably induced by (1) the formation of Mu^+-O^{2-} complexes with a polaronic electron at the Y cation and (2) the formation of metallic-like regions. The fraction of muonium at octahedral sites reduces by 9% under illumination, supporting the picture that, similarly, hydrogen is removed from these sites by the UV illumination.

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F2. Defects in thin films (semiconductors, oxides..)

Defect landscape in TiO_2 after ms-range annealing and resulting photocatalytic efficiency

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Transition metal oxides, particularly TiO_2, are photoactive materials, which can be utilized to clean the air from pollutants and to produce green hydrogen for clean energy at the same time. They are one of the most promising candidates for high-performance photocatalysis. In this work, we investigate the effect of 20 ms flash lamp annealing (FLA) of sputter deposited TiO_2, where arising from the light irradiation structural modifications of the films facilitates the photocatalytic (PC) degradation of two chemical compounds, namely methyl blue and methyl orange, once they interact with the surface of TiO_2. The precise control of the flash energy input enables tuning of the TiO_2 phase formation starting from pure anatase to mixed anatase/rutile phases, the latter associated with increased PC effect. Scanning electron microscopy and X-ray diffraction studies show that the crystal size and film quality increase with increasing annealing temperature. Further, the evolution of structural defects after FLA has been assessed by positron annihilation spectroscopy (PAS) and photoluminescence. Positron annihilation lifetime characteristics, i.e., positron lifetimes and their relative intensities profoundly sketch a transition between pure anatase and emerging rutile phase as a function of flash energy. Vacancy complexes close to the size of trivacancy dominate the anatase phase, whereas in the mixed anatase/rutile phase smaller open volume is evidenced, likely as a direct consequence of annealing. Finally, Doppler broadening PAS indicates the overall reduction of defect density exhibiting a similar transient phase region at the intermediate flash energies.

Tungsten-oxide thin films characterized by Positron Annihilation Spectroscopy

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For future nuclear fusion reactors it is foreseen that tungsten is used as inner wall cladding. Understanding the formation and behaviour of radiation induced defects in tungsten is therefore important for their safe operation. Tungsten mono-crystal model systems are studied by positron annihilation Doppler-broadening spectroscopy (DBS) and positron annihilation lifetime spectroscopy (PALS) to foster the understanding of the type and evolution of these defects. Both methods are sensitive tools when examining the defect type and concentration. However, data obtained by either of these methods is influenced by any thin oxide film on the surface of a sample. Such a film is present on any tungsten sample exposed to air, therefore its effect on DBS and PALS results needs to be known for their correct interpretation. In this work we measured tungsten-oxide thin films grown by thermal and electro-chemical methods as well as by exposure to air by DBS and PALS. The DBS measurements were performed using a tungsten-moderated β^+-emitter (Na-22) in a slow positron beam setup at MLZ that can achieve acceleration energies of up to 40 keV. The PALS measurements were performed at the accelerator-based MePS device at the positron source of ELBE at HZDR.

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F3. Defects in thin films (semiconductors, oxides..)

MePS – the Mono-Energetic Positron Source for annihilation lifetime spectroscopy

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The Helmholtz-Center Dresden - Rossendorf operates several user beamlines for materials research using positron-annihilation energy and lifetime spectroscopy. The superconducting electron linear accelerator ELBE drives several secondary beams including hard X-ray production from electron-bremsstrahlung, which serves as an intense source of positrons by means of pair production. The Mono-energetic Positron Source MePS [1] utilizes positrons with variable kinetic energies ranging from 0.5 to 18 keV for depth profiling of atomic defects and porosities on nm-scales in thin films. High timing resolutions (σ_t ≈100 ps) at high average event rates in excess of 10^5 s^{-1} and adjustable beam repetition rates allow performing high-throughput positron annihilation lifetime experiments. Acquiring an annihilation lifetime spectrum with 10^7 events takes about 80 s which paves the way to perform in-situ PALS experiments on dynamical defect evolution, migration and annealing [2,3,4].
We will present the actual status of the MePS facility and updates which are on the way. A recently constructed sample chamber will allow for fast and automated sample transfers, an increased sample temperature range (80 K to 800 K), and possibilities for sample illuminations with light sources (LED, Laser, and a broadband short arc Xe light source).
The facility is part of the ELBE Center for High-Power Radiation Sources which operates several secondary beam lines for international users.

The MePS facility has partly been funded by the Federal Ministry of Education and Research (BMBF) with the grant PosiAnalyse (05K2013). Trans-national access is available through the EU-Horizon project ReMADE for academic and industry.

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Point defects in GaN films deposited by metalorganic vapor phase epitaxy

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The development of short wavelength optoelectronic devices put an increasing demand on production of high quality GaN films. Metalorganic vapor phase epitaxy (MOVPE) is the most common technique for growing of epitaxial GaN layers. Electrical and optical properties of GaN films are governed by point defects. In the present work variable energy positron annihilation spectroscopy (VEPAS) was employed for characterization of vacancies in GaN layers grown using MOVPE at various temperatures. The GaN films were grown from triethyl gallium precursors up to 950°C and from trimethyl gallium precursors at higher temperatures. Influence of reactor atmosphere (N_2 or H_2) was investigated as well.

Obtained results showed that MOVPE deposition parameters, i.e. atmosphere in the chamber and precursor, affect point defects in GaN layers. However, the deposition temperature is the most important parameter determining type and concentration of vacancies in GaN layers. Interestingly. the dependence of V_{Ga} concentration on the deposition temperature is not monotonous. The lowest V_{Ga} concentration was observed in films deposited at 950°C. For higher deposition temperatures [V_{Ga}] increases in films deposited both in N_2 and H_2 atmosphere. At temperatures below 950°C GaN layers deposited in N_2 atmosphere contain higher [V_{Ga}] than films deposited in H_2 atmosphere.

Comparison of VEPAS results with photo-luminescence measurements revealed that [V_{Ga}] is correlated with the intensity of excitonic luminescence. Hence, GaN films with the highest V_{Ga} concentration surprisingly have the best optical properties. Since there is no known mechanism how V_{Ga} presence would enhance free-exciton emission, we suggest that the presence of V_{Ga} suppresses formation of yet unknown non-radiative centra in GaN. On the other hand, the intensity of defect-related yellow emission band (YB) is uncorrelated with V_{Ga} concentration testifying that V_{Ga} are not responsible for YB luminescence. The effect of post-growth annealing of GaN layers in various atmospheres was investigated as well.

Millisecond Flash Lamp Curing for Porosity Generation in Thin Films

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Flash lamp annealing (FLA) with millisecond pulse duration is reported as a novel curing method for pore precursor's degradation in thin films. A case study on the curing of dielectric thin films is presented. FLA-cured films are being investigated by means of positron annihilation spectroscopy and Fourier-transform infrared (FTIR) spectroscopy in order to quantify the nm-scale porosity and post-treatment chemistry, respectively. Results from positron annihilation reveal the onset of formation of porous voids inside the samples at 6 ms flash treatment time. Moreover, parameter adjustment (flash duration and energy density) allows for identifying the optimum conditions of effective curing. Within such a systematic investigation, positron results indicate that FLA is able to decompose the porogen (pore precursors) and to generate interconnected (open porosity) or isolated pore networks with self-sealed pores in a controllable way. Furthermore, FTIR results demonstrate the structural evolution after FLA, that help for setting the optimal annealing conditions whereby only a residual amount of porogen remains and at the same time a well-densified matrix, and a hydrophobic porous structures are created. Raman spectroscopy suggests that the curing-induced self-sealing layer developed at the film surface is a graphene oxide-like layer, which could serve as the outside sealing of the pore network from intrusions.

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Study of the memory effect in photochromic rare-earth oxyhydride thin films during multiple UV illumination cycles

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Rare-earth oxyhydride thin films show a color-neutral, reversible photochromic effect at ambient conditions, induced by illumination above the optical band gap. In this study, we report the evolution of the photochromism as a function of multiple illumination-bleaching cycles. For both YH_xO_y and GdH_xO_y, the photochromic contrast remains fairly constant, while the bleaching time shows a significant increase during the first four cycles, after which it remains constant. In order to gain an understanding of this memory effect, in-situ illumination Doppler broadening positron annihilation spectroscopy (DB-PAS) and positron annihilation lifetime spectroscopy (PALS) were employed. The DB-PAS study shows that the S-parameter increases during the first four illumination cycles and stabilizes upon further cycling for both YH_xO_y and GdH_xO_y thin films. The observed correlation between the S-parameter and bleaching time suggests that the formation of open volume defects may contribute to the origin of the memory effect. The in-situ PALS study on YH_xO_y thin films shows that both the shortest and the ortho-positronium (pick-off) lifetime components are significantly changed after bleaching. The intense short component, that was assigned to Y monovacancies in as-deposited YH_xO_y films, increases by more than 10 ps after bleaching, suggesting the formation of di-vacancies. Furthermore, the clear increase in the pick-off lifetime after bleaching indicates that nanopores are affected by the photochromic cycle. Finally, the reversible part of the shifts in the S-W point under illumination correlates with the photochromic changes in transmittance, and points to the formation of metallic-like domains [1]. Such formation of metallic-like domains is also consistent with the optical parameters after illumination as derived from spectroscopic ellipsometry.

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F4. Defects in thin films (semiconductors, oxides..)

Ab initio calculations of Positron lifetimes and the comparison with lifetime measurements in photochromic YH_xO_y thin films

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Rare-earth oxidyhydrides, such as YH_xO_y, show a reversible photochromic effect. However, the details of the underlying mechanism are not yet fully understood. A major influence on properties such as band gap, electrical conductivity or light absorption is achieved by modifying the chemical composition, i.e. the O^{2-} and H^- content of the material. Recently published results [1] of PALS measurements performed with the Pulsed Low-Energy Positron System (PLEPS) [2] on magnetron sputtered Yttrium-based thin films (Y, $YH_{\sim 1.9}$, YO_xH_y, Y_2O_3) report the occurrence of different positron defect lifetimes in the materials. Very often, such results are difficult to interpret because, especially in complex materials, different defect types may lead to similar positron lifetimes.
Therefore, ab initio calculations, based on ABINIT [3] were performed for further interpretation. ABINIT is an open-source software suite that uses density functional theory (DFT) by means of a plane wave basis set and pseudopotentials. With an additional package [4], self-consistent field calculations can be performed to determine positron lifetimes on the basis of two component density functional theory (TCDFT) using the projector augmented-wave (PAW) method. For our calculations, we used both, the local density approximation (LDA) and the generalized gradient approximation (GGA) for the exchange-correlation functional.
The comparison of the calculations with the data from previous experiments shows a high degree of agreement. The lifetime components obtained with PLEPS can be clearly assigned to distinct defect types and, thus, help to provide accurate knowledge of the defect structures of the investigated materials. On the other hand, the possibility of comparison gives information about the accuracy of the calculation methods used (such as LDA and GGA).

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Calculation of positron characteristics at the Carbon/$LiCoO_2$ interface

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Lithium-ion batteries (LIBs) are extensively used in energy applications, and the cathode material plays a critical role in the overall performance of the battery. $LiCoO_2$ is a highly developed and extensively used cathode material in LIBs due to its excellent electrochemical performance since the late 1980s. Positrons can serve as a reliable quantum probe for monitoring the Li-ion mobility at the interface of electroactive materials and carbon, usually referred to as carbon black. The combination of positron annihilation spectroscopy and density functional theory (DFT) calculations is a powerful approach for the advanced characterization of materials, providing a highly accurate method [1]. The carbon/oxide interface is a crucial region for controlling the Li-ion mobility during the charge and discharge processes [2]. In this work, we use the parameter-free GGA method [1] to calculate the positron lifetime together with the positron density distribution (PDD) in a carbon coated $LiCoO_2$ heterostructure. Our computational results correspond well to experimental data, shedding the light on the interface interaction between carbon and LCO at the quantum level.

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G1. Detection of near surface defects in metals

Vacancy-Type Defects Just below Fracture Surface in Hydrogen Embrittlement of Ni by Positron Probe Microanalyzer

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In hydrogen embrittlement of pure Ni, grain boundary fracture is a characteristic feature. Hydrogen reduces the stacking fault formation energy, which is expected to lead to pile-up of dislocations near the grain boundaries and an increase in local vacancy density [1]. The aim of this study is to demonstrate the formation of localized high density of vacancies just below the grain boundary by comparing with the defects behaviour in the bulk in hydrogen embrittlement of Ni by positron annihilation lifetime spectroscopy (PALS). We propose that a positron probe microanalyzer (PPMA) capable of injecting a monochromatic positron beam with a diameter of 100 μm is applied to measure defects just below the grain boundary.

The PPMA installed using linac-based positron source at AIST was capable of positron lifetime measurements by pulsed intense positrons [2]. A focused positron beam diameter was estimated to be 150 μm with an injection energy of 8 keV (average depth of injection 550 nm). The counting rate was about 50 cps with a time resolution of 240 ps. Hydrogen charge was performed for 4 h at RT in a 5 % H_2SO_4 + 3 g/L NH_4SCN solution at a current density of 40 mA/cm^2 using a cathodic electrolysis method. The hydrogen charge depth was calculated to be 30 μm. The H-charged Ni fractured at 34 % strain and showed intergranular fracture in the H-charged layer.

In the uniformly strained region for the fractured Ni, conventional PALS measurement gave 317 ps lifetime component as well as 150 ps component due to dislocations. Hydrogen stabilizes a formation of vacancies and vacancy clusters have been found by straining in the hydrogen environment. On the other hand, longer-lifetime components of 440 ps and 189 ps were detected at the intergranular fracture surface by PPMA. In PPMA, the influence of the surface layer must be considered, and the annihilation lifetime in Ni oxide film was estimated to be 360 ps. Therefore this result indicated that larger vacancy clusters were formed just below the grain boundary. It is considered that dislocation pile-up takes place near the grain boundary, where vacancy-hydrogen complexes are accumulated, and much larger vacancy clusters are induced. We guess that hydrogen accumulates in the vicinity of the grain boundary through such a process, leading to the intergranular fracture.

In conclusion, the defect behaviour just below the Ni fracture surface was measured for the first time by PPMA and this method is very useful to investigate the fracture mechanism of metals.

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Hydrogen absorption in black Al films

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Black metals (BMs) with porous surface can be prepared by magnetron sputtering in carefully adjusted low pressure (~ 1 Pa) of nitrogen [1]. Surface of BM is completely black because incident light is almost completely absorbed in multiple scattering on inner surfaces of fractal-like system of cavities. Extremely high surface-to-volume ratio of BMs is favourable for absorption of gases.

Hydrogen absorption in black Al films was investigated in the present work. Hydrogenation of black Al film grown by magnetron sputtering was compared with that of conventional smooth Al film with mirror-like surface. Both black and smooth Al films were loaded with hydrogen gas at the pressure of 100 bar and temperature of 200^{o}C. The microstructure of virgin and hydrogen loaded black and smooth Al film was investigated by variable energy positron annihilation spectroscopy (VEPAS). In smooth Al films positronium (Ps) is formed on the surface only. Hence, the Ps contribution quickly disappears with increasing energy of incident positrons. On the other hand, in black Al films Ps is formed in the whole layer and the Ps contribution was observed for all positron energies. It testifies that black Al films contain nanoscopic porosity where Ps is formed and localized.

Hydrogen loading did not result in any significant changes in smooth Al films. This is in accordance negligible solubility of hydrogen in Al. In contrast, hydrogenation caused significant changes of black Al films demonstrated by an increase of the intensity of Ps contribution as well as the intensity of positrons trapped at defects. It indicates that hydrogen loading introduced very high concentration of vacancies into black Al film. Since vacancies in Al are mobile an ambient temperature, hydrogen-induced vacancies agglomerated into vacancy clusters and nanoscopic voids.

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Hydrogen susceptibility of polished pure iron

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Mechanical polishing represents a simple method to generate near-surface defects. In a hydrogen environment, this allows one to study the interaction between defects and hydrogen, which plays a major role in the hydrogen embrittlement [1]. Surface treatment on iron and austenitic stainless steels is known to cause a ductility reduction [2,3]. Although the formation of dislocation within ~5 μm from the surface is expected to enhance the near-surface hydrogen concentration [2], the origin at the atomic level of the relationship between the surface roughness and the hydrogen susceptibility is unknown.

In this study, we investigated the hydrogen susceptibility of mechanically polished pure iron, by measuring the ductility by tensile testing while hydrogen charging the samples by cathodic electrolysis. Positron lifetime measurements at 10% strain and after fracture using a ^{22}Na positron source and the slow positron beam (20 keV) at AIST were carried out to observe the change in hydrogen-related defects.

The lifetime measurements showed the formation of hydrogen-induced vacancy clusters, along with dislocations related to the surface treatment. In the 10%-strained samples, the positron lifetime of the vacancy clusters increased from 280 ps in the sample with the smoothest surface to 320 ps in that with the roughest surface. A similar trend was confirmed in the near-surface layers with the positron beam. In the fractured samples, the increase in the positron lifetime of the vacancy clusters was even larger (320 ps → 380 ps). These results indicate that the surface roughness promotes the vacancy clustering and this process is enhanced as the tensile strain becomes higher. In addition, the ductility was reduced as a result of the polishing, as the fracture strain declined from 18% to 10%. A positive correlation between the size of the hydrogen-induced vacancies and the hydrogen susceptibility was revealed for the first time.

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G2. Detection of near surface defects in metals

Dynamic study of Vacancy-Hydrogen dynamics using a high-intense slow-positron beam

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The Mono-energetic Positron Source MePS at the Helmholtz-Center Dresden-Rossendorf utilizes positrons with variable kinetic energies ranging from 0.5 to 18 keV for depth profiling of atomic defects and porosities on nm-scales in thin films [1]. High timing resolutions (≈ 210 ps FWHM) at high average event rates above 10^5 s^{-1} and adjustable beam repetition rates allow performing high-throughput positron annihilation lifetime experiments. Acquiring an annihilation lifetime spectrum with 10^6 events takes about 80 s which paves the way to perform PALS kinematic experiments on defect evolution, migration, and annealing.
Selected cases of defect kinetics in various metal systems will be presented to show the potential of a high-intense positron source. We will focus on hydrogen-induced vacancy defects and hydrogen trapping in metal-hydrogen systems like Nb [3, 4] and Ni [5]. Such systems are interesting from both a theoretical and a practical point of view. They are utilized for energy-storage systems, in sensor applications, and in catalysis. Most of hydrogen's interesting properties relate to the high mobility of the hydrogen atoms (similar to that of ions in aqueous solutions) due to occupation of interstitial positions in the host lattice. Open volume lattice defects (vacancies, vacancy clusters, dislocations), are known to have high trapping potential for interstitial hydrogen. Dynamic studies of the formation and evolution of surface-near vacancy-hydrogen defects help to understand the interactions between hydrogen and vacancy-defects and explain effects like hydrogen embrittlement processes or temperature-dependent defect stabilization. Since the time-scales of these defect dynamics are in the range of minutes to hours, kinematic defect studies can only be performed using a high-intense positron source like the MePS setup.

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In-situ positron lifetime measurements of pure iron during tensile deformation using gamma-ray-induced positron annihilation spectroscopy

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The mechanism of hydrogen embrittlement in steel is still unclear, and a model in which vacancies are involved in fracture has also been proposed [1]. Positron annihilation spectroscopy has also been used to study brittle-fractured samples [2]. However, the defects observed after fracture may differ from those formed before. Therefore, the use of in-situ measurement techniques is desirable to elucidate the contribution of defects to fracture. Gamma-ray-induced positron annihilation spectroscopy (GiPAS) allows the positron lifetime measurements of samples under environments difficult for the measures by a sealed radioisotope positron source. As a first step, we used the GiPAS technique at the UVSOR synchrotron facility [3] to observe defects formed during tensile deformation in pure iron. Dumbbell-shaped samples with a thickness of 3 mm were mounted on a small tensile tester and stretched up to a nominal strain of over 7% with a strain rate of 2.2×10^{-5} /s. The 3-mm-diameter gamma-ray beam for the electron pair creation in the sample was injected into the centre of the sample during tensile deformation to measure the change in positron lifetime. Ten samples were measured under the same tensile deformation condition to obtain positron lifetime spectra with sufficient counts. Preliminary results on the changes in positron lifetimes during tensile deformation will be presented on the day.

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Identification of vacancy-type defects in self-ion irradiated tungsten: A combination of experiments (PAS, TEM) and simulation

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Facing to energy shortage in the future, the thermonuclear fusion could be one of the key solutions to address the issue while reducing the greenhouse effect. On the fusion development roadmap, ITER and DEMO tokamaks are essential steps. And material behavior in such device is one of the challenges.

Tungsten was selected to cover the ITER divertor and is considered for the first walls in the Demonstration power plant (DEMO). Such components have to withstand high heat and particle flux. It is already known that under such severe operational conditions, material properties will be degraded. To dimension the reactor components, it is essential to predict precisely their impact and multi-scale modeling is used to simulate the effect of irradiation on the evolution of the microstructure and needs experimental data to be validated. For this purpose, we propose to combine positron annihilation spectroscopy (PAS) experimental and theoretical data as well as transmission electron microscopy (TEM) analysis to get the vacancy defects distribution induced in self-irradiated tungsten.

Tungsten samples were irradiated with 20 MeV tungsten ions which create damage in the first 1.6 µm approximately, and characterized by variable monoenergetic slow positrons. Doppler Broadening was recorded with the continuous beam installed in CEMHTI, and Positron Annihilation Lifetime was measured with the Pulsed low energy positron system (PLEPS) in Munich. Lifetime spectra show the detection of a new positron trap with a shorter lifetime compared to that of the single vacancy. Based on the vacancy cluster distribution obtained from TEM observation and the theoretical annihilation characteristics calculated by two-components density functional theory (TCDFT), a trapping model was applied to extract the momentum distribution of positron-electron annihilated pairs for the new positron trap. By comparing theoretical and experimental results, we propose that the new positron trap is probably mixed vacancy-impurity complexes.

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G3. Detection of near surface defects in metals

What we can learn from the statistical thermodynamics of point defects in metals

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Positron annihilation (PA) spectroscopy (PAS) is often used to investigate point defects, mainly vacancies, their small clusters and aggregates with other defects. The interpretation of PAS experimental data is generally tricky and usually relies on the previous experience of positroners and analogies with similar systems. Density functional theory (DFT) PA defect response calculations and simulations may help to predict and interpret measurements. However, this may not be enough to make a plausible explanation of measured spectra. On the other hand, statistical thermodynamics of point defects (STPD) based on DFT total energy calculations provides information about defect concentrations and say whether some defect types prevail over others. In addition, some defects may interact and effectively cause defect transformations, which is possible to incorporate into STPD studies. Metallic systems are easier to handle since the electron band structure does not need to be taken into account explicitly.

In order to get a complete overview of defects, not only vacancies but other types of defects need to be considered: antisites, interstitials and compound defects (e.g., vacancy-antisite pairs). Extensions to off-stoichiometric systems are also possible. The most suitable approach [1] is to use the generalized grand canonical thermodynamic potential and minimize it with respect to the number of different types of point defects under the constraint of constant composition of the system under study. In this way, the chemical potentials of atomic species can be determined. It is also possible to deduce whether the crystal disorder induced by the defects is due to antisites, vacancies or both. Detailed STPD examinations are elaborate and time-consuming. In this presentation, a few examples of intermetallics are discussed: FeAl, Fe_3Al [2], and the Heusler compound Mn_2FeSi [3]. STPD considerations are accompanied by positron lifetime calculations for vacancies in investigated compounds and discussed in terms of experimental data available.

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Microstructure of black metal films prepared by thermal evaporation

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Metals of highly porous surface feature usually significantly reduced reflectivity. Such metals are called black metals (BMs) [1]. BMs can be prepared by magnetron sputtering or thermal evaporation of a metal target in carefully adjusted low pressure (~100 Pa) of a gas not interacting chemically with metal atoms (usually N_2 or Ar) [2,3]. Deposition parameters leading to BM formation have to be determined experimentally for each metal. By decreasing gas pressure below ~1 Pa one can prepare also conventional metallic layer with mirror-like reflective surface in the same setup.

The surface of BM appears completely black despite the fact that corresponding reflective metal exhibits a high reflectance and a low absorbance for visible light. In contrast, the absorbance of BMs exceeds 90% in the whole wavelength range of visible light (350-800 nm). It is believed that BMs consist of fractal-like system of cavities having a broad size distribution. Then almost all incident light is eventually absorbed after multiple reflections on surfaces of these cavities, resulting in black appearance of the metals. However, detailed morphology of BMs is not completely understood yet.

In the present work the microstructure of black and reflective films of various metals (Al, Ti, Sb, Bi) deposited by thermal evaporation was investigated using variable energy positron annihilation spectroscopy (VEPAS) combined with electron microscopy. BM films were compared with conventional reflective layers of the corresponding metal grown in the same setup at low gas pressure.

VEPAS investigations revealed that in the reflective metal films positronium is formed at the surface only while in the BM films positronium is formed in the whole layer. It testifies that the BM films contain nanoscopic pores inside the layer which are not present in the reflective films.

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Coincidence Doppler broadening study of materials for supercritical water-cooled small modular reactors

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Despite undoubtful progress in developing new materials for harsh radiation environments, stainless steel with different grades is still one of the most promising structural materials for the next generation of nuclear power facilities, such as supercritical water-cooled reactors (SCWR). Along with improving high-temperature mechanical properties, substantial attention is dedicated to the corrosion properties of the candidate materials. The already high corrosion resistance of the stainless steels has been further improved in the alumina-forming austenitic (AFA) stainless steels, which are expected to provide superior oxidation resistance in SCWR conditions [1,2]. However, the pretreatment required for the formation of the alumina protective layer and the accompanying microstructural processes is still unclear.
In this study, the evolution of Al_2O_3 of Fe–24.8Ni–20Cr-2.0Al-0.5Nb-based AFA steel with different ageing times was investigated by slow positron beam annihilation coincidence Doppler broadening spectroscopy (CDBS). The results showed that a layer of Al_2O_3 oxide with a thickness of ~120 nm was formed on the surface of AFA steel air heat-treated at 850°C for 25 h. The structure and the chemistry of the surface layer were confirmed by comparing the CDBS curves of the AFA samples with/without heat-treated and the reference alumina samples. It was furthermore revealed that the formation of alumina, driven by the diffusion of Al from the bulk towards the surface, leaves behind vacancy-type lattice defects. Similar behavior was observed in the formation of the surface oxide films in 310S stainless steel and 800HT nickel-based alloy exposed to supercritical water and subsequently characterized by positron annihilation techniques and SEM-EDS. The results of this experiment confirm a slightly higher oxidation rate of alloy 800HT than 310S stainless steel. The presented study demonstrates the unique potential of the positron annihilation techniques based on slow positron beams in the experimental characterization of environmentally aged corrosion-resistant structural materials.

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Posters II

Causal relationship between hydrogen-induced defect formation behaviour and mechanical properties in austenitic stainless steels

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The hydrogen embrittlement (HE) of austenitic stainless steels used as hydrogen storage materials is one of the most serious issues to be solved in the coming hydrogen society. In austenitic stainless steels, the lower the Ni equivalent, the more likely the formation of a stress-induced martensitic (α') phase and the higher the HE sensitivity. We have applied positron annihilation lifetime spectroscopy (PALS) to investigate the vacancy behavior in ANSI 304 with high HE sensitivity [1-3]. In this study, we aimed to compare the hydrogen-induced defects among ANSI 304, 316, and 316L with different Ni equivalent by PALS and to obtain the causal relationship between the defect formation behaviour and mechanical properties.

The hydrogen charge was carried out by cathodic electrolysis. The electrolyte was 3% NaCl + 3 g/L NH_4SCN solution, and the charge was conducted at a current density of 50 A/m^2 at RT for 48 h. The H-charged specimens were strained by 10%, followed by the etching of the 10-μm thick hydrogen-charged layer. Two types of specimens were prepared: one was etched immediately after straining (non-aged specimen), while the other was aged at RT for 4 days after etching (aged specimen).

The PALS results showed bulk lifetime and about 180 ps components in all non-aged specimens. Since this lifetime was longer than that due to dislocations, it was attributed to defects consisting of a mixture of dislocations and monovacancies. As monovacancies are unstable at room temperature, they are expected to be bound with hydrogen (vacancy-hydrogen complexes). On the other hand, in the PALS for all the aged specimens, vacancy cluster formation more than 200 ps was observed. The desorption of hydrogen during aging for 4 days induced the diffusion and aggregation of vacancies, followed by a formation of vacancy clusters.

None of the aged specimens showed any ductility loss, but the non-aged specimens of ANSI 304 and 316 showed ductility loss, while ANSI 316L did not. Although vacancy-hydrogen complexes were formed in the non-aged specimens of ANSI 316L, the γ-phase is stable and the formation of high strain fields is considered to be less likely. In contrast, in the non-aged specimens of 304 and 316L the growth of vacancy clusters was observed at fracture. It is suggested that the agglomeration of vacancy-hydrogen complexes in high concentration at the α' phase boundary, which is a high-strain field, may be responsible for HE in ANSI 304 and 316.

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LT-Upscaler
An approach to enable in situ measurements on a laboratory scale

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The LT-Upscaler is a software to upscale Positron Annihilation Lifetime measurements with low statistic to spectra with high statistics. In this work we validate the functionality of the LT-Upscaler with simulated Lifetime spectra with known Ground Truth. Therefore, a Lifetime Spectra with source and two other components are simulated. The components and the respective intensity of the two components change over time.

Measurement of the positronium 2^3P_J fluorescence decay rate

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Measurements of positronium (Ps) decay rates can be used to test QED theory [4], and contribute to the search for new physics. Annihilation decay rates have been measured for the ground states [1,2] and the 2^3S_1 excited state [3] of Ps. Here we report a measurement of the fluorescence decay rate of Ps atoms in the 2^3P_J level, using a new technique. An electric field was applied to metastable 2^3S_1 Ps to produce Stark-mixed states, consisting of both 2^3S_1 and 2^3P_J components. The relative population of these components was controlled by varying the strength of electric field applied. At a later time a larger electric field was applied to induce rapid quenching and annihilation of these mixed states. The number of quenched atoms for a range of mixing field strengths was measured, from which the effective decay rate of the mixed states, and so 2^3P_J state, can be obtained. The result is consistent with theory, but does not have a precision sufficient to test QED. We discuss possible improvements to the methodology that could allow for a more precise measurement.

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Defect profiling using diffusion and non-diffusion trapping model - e^+DSC code

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Profiling defects near the surface of a solid with slow positrons is an important research area of positron spectroscopy. The 1D diffusion trapping model is successfully used to describe experimental data. This model takes into account the profile of positron implantation and the diffusion of thermalized positrons. The poster will present the method and solution of the rate equations of this model based on the Green's function. They have been implemented into the e^+DSC (positron Depth SCanning) computer code [1]. This code will be presented along with some positron beam results.

The 1D trapping model assumes positron diffusion, this requires a homogeneous and rather small concentration of defects to allow them to random walk. But under certain conditions it is conceivable that the concentration of defects is so high that each positron is trapped immediately after thermalization, i.e. trapping saturation occurs. This is observed, for example, in metals or alloys that are strongly plastically deformed. It can be assumed that the saturation may be different at different depths, e.g. the type of defect may be different at different depths. In this case, diffusion is almost impossible.

Then, the non-diffusion trapping model will also be presented in the poster. This model is able to describe the confusing results obtained in a slow positron beam, which will be demonstrated in the examples.

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Positron diffraction stations at the Slow Positron Facility in IMSS, KEK

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At the Slow Positron Facility [1] in the Institute of Materials Structure Science, KEK, stations for the total-reflection high-energy positron diffraction (TRHEPD) [2, 3] and the low-energy positron diffraction (LEPD) [3] are in operation for the detailed analysis of the surface atomic arrangements. Also in operation are a general purpose experiment station (currently used for Ps laser cooling experiments) and Ps time-of-flight experiment station. The stations are open to external users through the approval of their research proposals.

The slow positron beam is created with a Ta/W converter/moderator from an electron beam accelerated to ~50 MeV by a dedicated electron linear accelerator. The slow-positrons are then accelerated to the energy required by an individual experiment and transferred magnetically to the area of the experiment stations.

The lineac is operated at 50 Hz in two pulse modes; a long-pulse mode with a width of 1 μs and an intensity of $\sim 1 \times 10^8$ slow-e^+/s, and a short pulse mode with a width of ~10 ns and an intensity of $\sim 1 \times 10^7$slow-e^+/s. The diffraction experiments use the long pulse mode beam.

TRHEPD is the positron counterpart of RHEED. The beam is transported at an energy of 15keV, brightness-enhanced with a W-foil remoderator near the experiment station, and transported at 10 keV in the magnetic-field-free region to the station. Sample surfaces are prepared inside the measurement station, or in an independent preparation chamber located in the same experiment hall and transferred to the experiment station with a portable UHV transfer-vessel.

LEPD is the positron counterpart of LEED. The beam is transported at an energy of ~5 keV, brightness-enhanced with a single crystal Ni-foil remoderator near the experiment station, and transported at an energy ranging from a few tens of eV to a few hundred eV in the magnetic-field-free region to the station. Since LEPD patterns are detected by a position sensitive delay-line-detector (DLD) which works properly only when the time separation of consecutive incident positrons is above a limit, the beam pulse is stretched to increase the separation before reaching the remoderator [5]. Sample surfaces are prepared in an independent sample preparation chamber, which is connected to the the experiment station but isolated with a gate valve except during sample transfer [6].

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Investigation of hydrogen incorporation in Zr-ion implanted Zircaloy-4 using positron annihilation lifetime spectroscopy

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Most commercial reactors are light water reactors use zirconium-based alloys to contain the uranium oxide in the fuel rods. An important mechanism for in-reactor corrosion of Zr-based fuel claddings is hydrogen uptake (pick-up) which may induce cladding embrittlement [1]. Hydrogen that diffuses into the metal may be found either in solid-solution in the α-Zr matrix or, if the hydrogen concertation is high enough, as Zr-hydride. The fraction of free hydrogen increases with temperature. In this study 800 MeV self-ion, Zr-ion, implantation of zircaloy-4 samples was used to create a vacancy-related defect profile with a peak at approximately 150 nm. Samples containing ambient hydrogen and hydrogen-charged (100 wt. ppm) samples were studied. To investigate the possible incorporation of hydrogen at vacancy related defects variable energy positron annihilation lifetime measurements were performed using the mono-energetic positron source beamline at Helmholtz–Zentrum Dresden–Rossendorf. Previous studies have demonstrated the capability of the method to study hydrogen vacancy interactions [2]. As-received and H-charged samples were studied along with uncharged and H-charged samples subjected to varying Zr-ion implantation fluences. Measurements on selected samples were performed between 50 °C and 280 °C to investigate the effect of increasing the fraction of free hydrogen. In this work the results from these measurements will be presented and discussed.

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Effect of foreign interstitials to irradiation damage in equi-atomic FeMnNiCoCr high entropy alloys

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High entropy alloy, or multi-principal element alloy, have gained particularly strong research interest in recent decades [1-2]. Some of the HEAs shown outstanding irradiation tolerance, which have the potential to be developed as structural materials and service in extremely harsh environment. In this work, we carried out 480 keV helium ion implantation to equi-atomic FeMnNiCoCr with and without C/N interstitials at room temperature, 473K and 573 K, respectively. Doppler broadening spectroscopy based on slow positron beam have been applied to characterize the irradiated samples. Conventional S and W parameters have been extracted from the Doppler broadening spectra. The results indicated that certain amount of vacancy defects formation in irradiated samples. Vacancy clusters were formed in the 573K irradiated samples. C and N interstitials addition in the HEA suppressed the damage production. They also prohibited vacancy clustering significantly in high temperature irradiated samples.

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Hydrogen-induced defects in TiO_2 films covered with catalytic Pd layer

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Palladium is widely used for catalysing hydrogenation reactions since on Pd surface H_2 molecule is easily dissociated into atomic hydrogen [1]. Recent experimental and theoretical studies have demonstrated that the presence of subsurface hydrogen significantly influences the reactivity and selectivity in the hydrogenation processes [2]. Rutile (TiO_2) is frequently used as a support of metallic layers in various metal/oxide devices, e.g. gas sensors. The aim of the present work was investigation of the influence of hydrogen gas on TiO_2 covered with thin (200 nm) Pd over-layer.
Combination of variable energy slow positron annihilation spectroscopy (VEPAS) and environmental transmission electron microscopy (ETEM) revealed that microstructural changes in Pd layer deposited on TiO_2 strongly depend on the partial hydrogen pressure in the environment atmosphere. Formation of superabundant vacancies was observed in the Pd layer at hydrogen pressure above 0.01 mbar with concentration gradually increasing up to 1.6×10^{-4} at.$^{-1}$. Further increase of hydrogen pressure above 1 mbar introduced dislocations formed due to mechanical stress arising between the Pd layer and TiO_2 substrate. Both vacancies and dislocations act as positron traps. At hydrogen pressure of 100 mbar hydrogen induced stress exceeds the adhesion of Pd film to the substrate and the Pd layer is detached from the substrate. Hydrogen penetrating into TiO_2 substrate and trapped in Ti vacancies was observed at hydrogen pressure of 100 mbar.

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Microwave Spectroscopy of the Positronium fine structure and Rydberg Helium

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Previous measurements of the positronium (Ps) fine structure using microwave spectroscopy [1], made in both free-space and in waveguides were found to be susceptible to line shape distortions arising from reflected microwave radiation [2], which in turn resulted in large apparent frequency shifts. New waveguide measurements designed to mitigate these effects allowed for increased precision and accuracy, but still exhibited a frequency shift. Such experiments may be used to test QED but are presently much less precise than theory [3]. Here we describe a new technique in which microwave spectroscopy of dressed Rydberg He atoms is used to characterize the electric field in a waveguide [4] and address the discrepancies between the theoretical and experimental values in Ps.

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P20- The convoluting spectrum analysis of the positron lifetime in molybdenum (_42^96)Mo into several spectra such as FWHM, ESG, background, and radioactive isotope (22Na) using PALSfit, Scilab-6.0.1 programs.

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*Speaker

A positron trap for observing molecules containing positronium

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A positron trap is a powerful and adaptable tool for performing experiments with positrons and positronium. These devices use a strong magnetic field, a stepped potential well and Nitrogen and CF_4 buffer gas. Positrons are initially trapped via the electronic excitation of N_2, CF_4 is added for efficient cooling via vibrational and rotational excitations. This type of positron trap can typically produce ~10^5 e+/s in bunches with a diameter of 1-2 mm and an energy spread of approximately 50 meV [e.g. 1,2].

We aim to use the positron pulses from such a trap to observe molecules containing positronium, such as PsH [3] and PsO [4] via collisions in gases such as methane and carbon dioxide. By using a high mass resolution ion spectrometer to detect fragments from dissociation, precise measurement of their binding energy will be performed.

This poster will describe the positron beam, trap, and ion spectrometer and show first trapping results from the newly constructed positron beamline in Vienna.

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[3] D.M. Schrader, F.M. Jacobsen, N.-P. Frandsen, U. Mikkelsen, Formation of positronium hydride, Phys. Rev. Lett. 69 (1992) 57–60.
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Doppler-broadened variable-energy positron annihilation spectroscopy of luminescent Eu-doped SiN thin films.

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Light emission has always been a significant area of interest for silicon-based photonic devices. Several approaches have been developed to enhance the performance of devices, including doping with rare-earth elements, such as Europium (Eu). Eu has two optically active states, Eu^{2+} and Eu^{3+}, which leads to a wide range of light emission from the red to blue spectral region. Thus, such material is promising for solid-state light emission applications, such as light-emitting diodes (LEDs) and lasers.

In this study we have investigated four sets of Eu-doped SiN_X thin film samples which were fabricated via combined electron cyclotron resonance-plasma enhanced chemical vapor deposition (ECR-PECVD) and magnetron sputtering, with different nitrogen concentrations and subjected to different annealing temperatures post-deposition. Optical performance was characterized via photoluminescence spectroscopy (PL), while multiple materials characterization techniques including Doppler-broadened variable-energy positron annihilation spectroscopy (VEPAS), and Rutherford back-scattering spectrometry (RBS) were used to gain more insight into the luminescence mechanism(s). This talk will present some of the resulting data, with a focus on VEPAS, to illustrate these mechanisms.

He trapping in H+ Irradiated Polycrystalline Tungsten Samples: A Combined Study Using Positron Annihilation spectroscopy and Nuclear Reaction Analysis

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Tungsten is considered as a propitious plasma-facing material in fusion reactors. The trapping behavior of particles such as helium and H-isotopes -the product and the fuel of the fusion reaction respectively- in tungsten is crucial in view point of efficiency and safety of fusion device operation. Present study is focused on the helium (^{3}He) trapping in pre-damaged polycrystalline tungsten using 2.8MeV proton (H^+) irradiations. Before proton irradiation the tungsten samples were annealed at 1700 °C for 3 hours and examined by positron annihilation spectroscopy (using SPBDB - slow positron beam coupled with a Doppler broadening spectrometer). The results confirmed the vacancy defects were annealed out. Then the samples were irradiated with 2.8MeV protons for different fluences (5×10^{15} cm^{-2}, 4×10^{16} cm^{-2}) and the induced vacancy defect distribution were characterized using SPBDB. Subsequently, the proton irradiated samples were exposed to ^{3}He plasma at a low flux of about 10^{12} cm^{-2}-s^{-1}. Then SPBDB is used to analyse the vacancy defect distribution after He exposure and specifically the helium trapping in vacancies. In parallel the introduced and remained ^{3}He fluences were determined by nuclear reaction analysis (NRA) in the exposed tungsten samples. The effect of ^{3}He exposure fluence on the vacancy distribution is investigated as well as the impact of the presence of vacancies before exposure on the retained He quantity and on the He-vacancy complexes distribution.

21-21 Jul 2023

H1. Prospects

Toward materials science using an energy-tunable Ps beam in the energy range of a few keV

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Using photodetachment of Ps^- accelerated by an electric field, an energy-tunable Ps beam of a few keV has been developed and used in several studies [1-4]. Ps can be regarded as neutralizing particles of electrons and positrons, and their properties as neutral particles with much lower mass than hydrogen atoms are expected to be used for applied research. Unfortunately, the current Ps beam intensity is lower than that of typical slow positron beams. However, if the intensity is improved, it may be possible to use Ps beams instead of slow positron beams for depth profiling [5] and crystal surface analysis [6], which have been performed with slow positron beams. This method is expected to enable more accurate measurements of easily charged insulators and magnetic surfaces [7].
Currently, we are conducting experiments to investigate the quantum interference effects of Ps and to measure the efficiency of Ps transmission through graphene. In this presentation, we will discuss these preliminary results and future prospects.

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Development of gamma-ray-induced positron annihilation spectroscopy at UVSOR-III

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Inverse Thomson/Compton scattering is a scattering process between high energy electrons and laser photons, which can produce high energy gamma rays. For example, a MeV gamma ray can be generated by the scattering between a 1 GeV electron and a 1 eV photon. The generated gamma rays possess features such as quasi-monochromatic and tunable energy, high polarization, and low divergence angle. Pulsed gamma rays are generated by scattering of electron beam bunches and pulsed lasers. Ultra-short pulsed gamma rays have been developed by 90 degree inverse Thomson scattering between a 750-MeV electron beam and a Ti:Sa laser pulse at the synchrotron radiation facility UVSOR-III in Japan [1]. The maximum gamma-ray energy is 6.6 MeV and the pulse width is calculated to be sub-ps to ps ranges.

The ultra-short pulsed gamma rays were applied to gamma-ray-induced positron annihilation spectroscopy. In gamma-ray-induced positron annihilation lifetime spectroscopy (GiPALS), a positron lifetime measurement system with a time resolution of 140 ps in full width at half maximum was developed using eight BaF_2 detectors and two digital oscilloscopes (DSO). GiPALS is currently available for users and in situ measurements of positron lifetime under stress loading is conducted [2]. The development of gamma-ray-induced age-momentum correlation (GiAMOC) using two DSOs and two BaF_2 detectors is also in progress [3]. In addition, the effect of coincidence detection of Compton scattered and annihilation gamma rays on positron lifetime spectra is calculated using the Monte Carlo simulation code EGS5. In this conference, the current status of these studies and future plans, including the development of spin polarized positron annihilation spectroscopy using circularly polarized gamma rays, will be presented.

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Positronium interferometry to measure the effect of gravity

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The gravitational acceleration of antimatter has not been measured until now. Shedding light on this new knowledge may open new frontiers for understanding hitherto unexplained phenomena, such as the accelerated expansion of the Universe. Positronium (Ps) has been proposed by QUPLAS collaboration [1] as a test to measure the effect of gravity. In this work, we propose the use of positronium interferometry to measure the gravitational acceleration of antimatter. Our approach is to prepare a Ps beam forming a continuous, monoenergetic negative Ps ion (Ps-, i.e. the bound state of two electrons and one positron), then remove the extra electron using a Fabry-Perot IR laser cavity and excite Ps to the long-lived n=2 state using a second UV laser. After Ps beam formation, the strategy is to use a Mach-Zehnder matter-wave interferometer operating with optical gratings in single-photon transitions mode [2]. This method could provide a unique tool to test the weak equivalence principle. The work shows the calculated characteristics of the Ps beam and the operating parameters of the interferometer.

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H2. Prospects

Positronium density measurement technique using Polaritonics

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Positronium (Ps) is an electron-positron bound state forming in fact a meta-stable two-body atomic system. As Ps is bosonic, a long term goal of Ps physics has been the formation of an ensemble of Ps atoms cold/dense enough to create a Bose-Einstein Condensate (BEC). Its primary motivation is that such a system may exhibit the phenomenon of stimulated annihilation [1], allowing for the creation of a gamma-ray laser.

Recent experimental advances in Positronium physics have made it possible to produce dense Ps ensembles confined within the voids of porous materials, paving the way to the realization of a Ps BEC [2]. In order to achieve this latter goal it would be advantageous to develop new methods to measure Ps densities in real-time. Here we describe a possible approach to do this exploiting concepts of cavity quantum electrodynamics (CQED) [3], the field that investigates the interaction between dipolar active transitions in atoms, molecules or other materials, and single photons inside an optical cavity. When the light-matter coupling strength becomes larger than the loss rates of the light and matter excitations, the system enters the so-called *strong coupling* (SC) regime, and it can be described only in terms of the light–matter hybrid eigenmodes of the coupled system, often named *polaritons* [4, 5]. Using realistic experimental parameters we demonstrate that a dense Ps gas, can be strongly coupled to the photonic field of a distributed Bragg reflector microcavity [4]. In this strongly coupled regime, the optical spectrum of the system is composed of two hybrid Ps-polariton resonances separated by the vacuum Rabi splitting, which is proportional to the square root of the optically active atoms, and as such can serve as a direct measurement of the Ps density. This phenomenology is demonstrated for the $1S \leftrightarrow 2P$ optical transition [6] in the UV spectrum by employing AlGaN/AlN DBRs [7], and for transitions between Rydberg states ($n > 10$) coupled to a high-quality-factor DBR cavity in the mid- to far-infrared range [8]. Given that polaritons can be created on a sub-cycle timescale, a spectroscopic measurement of the vacuum Rabi splitting could be used as an ultra-fast Ps density measurement in regimes relevant to Ps BEC formation.

Moreover, we show that Ps-polaritons could also enter the ultrastrong light-matter coupling regime [10] potentially exhibiting its rich phenomelogy, such as the presence of virtual excitations in the ground state and the possibility of modifying the Ps wavefunction [9].

In conclusion, the new found connection between positronium research and polaritonics not only solves one important problem in the path towards the achievement of Ps BEC, that is the ultrafast real-time measurement of the Ps population, but also offers to polaritonic scientists the unique opportunity of exploring non perturbative light-matter phenomena on a novel powerful polaritonic platform.

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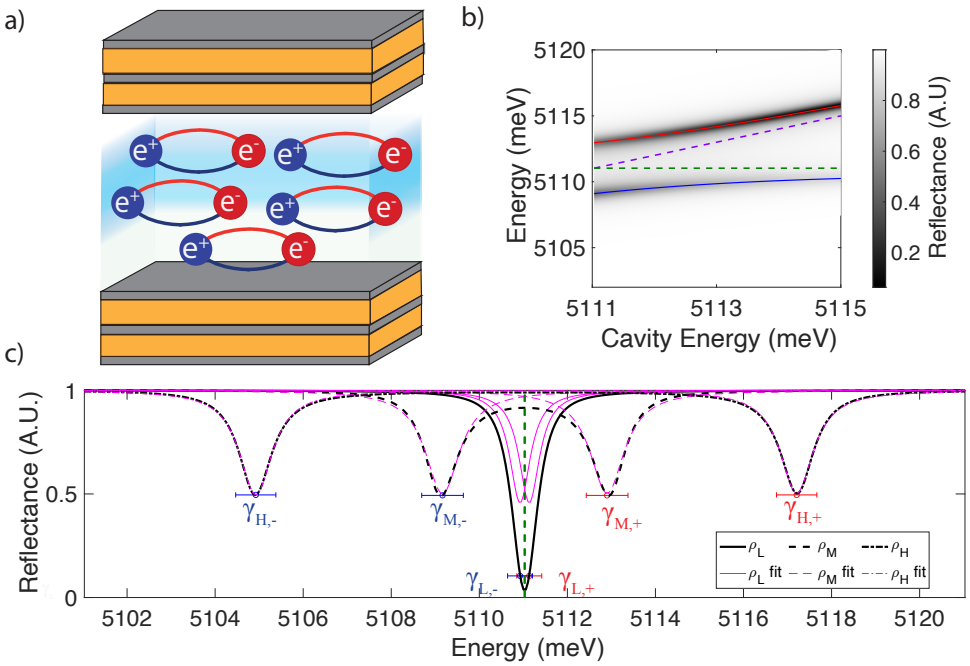

FIG. 1. (a) Sketch of Ps CQED system, representing Ps atoms interacting with the electromagnetic field trapped in a cavity formed by two DBRs.(b) Reflectance spectra of the cavity-Ps system as function of the bare cavity frequency (violet dashed line), calculated via transfer matrix at the Ps atoms density of 10^18 cm^{-3}. (c) Reflectance spectra at the resonance condition (black dashed line) at densities of 10^16 cm^{-3}. 10^18 cm^{-3}, 10^19 cm^{-3}. The polaritonic resonances have been fitted by Lorentzian functions (magenta lines) from which the linewidths of the different resonances have been extracted

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Graphene-based atto-amperemeter positron sensors

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We report the development of charge-sensitive devices aimed to complement PAS methods by detecting the charge left at the wake of positron annihilation events. Our method is based on the fabrication of graphene field-effect transistors which are used as sensitive charge probes, sensing the charge which builds up in floating charge accumulation elements [1,2]. In the talk, we will report on two generations of devices. First is a DC-operated device, where charge accumulation is detected by tracing the charge-neutrality condition in the graphene channel. The DC devices reach a sensitivity of 1.2 fA/√Hz [2]. We will then report on our newer generation RF devices, reaching a sensitivity of 0.01 fA/√Hz, corresponding to ~100 positrons/sec. In these RF graphene-based devices, the graphene is coupled to a waveguide and is integrated as an RF resonator, where annihilation events are detected through changes in the graphene RF-reflection coefficient S_{11}. We expect our detectors to be useful in singling out layer-specific information, in particular detecting positrons annihilation within thin films, once the detectors are integrated within our positron beam [3]. Furthermore, the RF detectors are designed with a vision of detecting individual positrons and correlating charge signatures with gamma annihilation events. This, in turn, would allow us to identify annihilation signatures from localized regions in a sample.

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