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Papers

Digital Positron Lifetime Spectrometer

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The advent of extremely fast (> 1 GS/s) analog-to-digital (ADC) converters has allowed measuring the positron lifetime digitally [1-3]. The basic idea of the approach is to directly digitize the detector anode pulses and to perform the timing with software, thus completely skipping the analog electronics chain.

Our digital lifetime spectrometer consists of a fast commercial digitizer (Acqiris DP210, 2 GS/s, 8 bit, 500 MHz) connected to a computer, a simple coincidence circuit and software to extract the timing information from the digitized detector pulses. The performance of the system is equal to that of an analog spectrometer with similar detectors; with $\phi 30 \times 20$ mm^2 plastic scintillators the obtained time resolution is 220 ps (50% ^{22}Na energy windows). Also, the count rates achieved with the system are similar to those of the analog spectrometers, typically around 250 1/s. The pulse processing part of the system is capable of storing and processing several thousands of events per second in real time.

The programming approach allows to use several timing algorithms, many of which are in practice impossible to implement with analog electronics. We found that the most effective timing algorithm is to fit a smoothing spline curve to the leading edge of the anode pulse. Timing of the pulse is then accomplished by constant fraction principle from the fitted curve. The digital approach has many advantages over the analog one, e.g. minimal number of components, no tuning of timing electronics, inherent linearity, stability and versatility.

[1] K. Rytsölä, et. al., *Applied Surface science* 194, 260 (2002).
[2] H. Saito, et. al., *Nucl. Instr. and Meth*. A 487, 612 (2002).
[3] J. Nissilä, et. al., submitted to *Nucl. Instr. and Meth*. *A*.

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Positronium Imaging in Positron Emission Tomography

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In this work, we investigate the potential use of positronium decays into three-photon positron annihilation processes for positron emission tomography (PET) applied in medical diagnosis. Positronium annihilation into three photons would provide information not only about the local concentration of a radionuclide, but also, its local chemical environment in tissues. In particular the level of free oxygen in tumours may be determined, which can be a significant advantage in applications of PET to oncology. PET is a functional imaging modality with a unique role because it uses radioactive short-lived forms of organic species such as ^{11}C, ^{13}N, ^{15}O, and ^{18}F which are isotopes of important body elements. At present, PET as a diagnostic imaging technique is based on the predominant 2γ positron annihilation process. However, the detection of 3γ annihilation photons carries much more information about the environment with which the positron interacts. The rate of positronium decay is proportional not only to the local concentration of the radionuclides but also to the yield of 3γ annihilation. This in turn depends on the local chemical environment. The paper presents the results of experiments in imaging point-like sources and measurement of the yield of 3γ annihilation events, registered by a system comprising three high energy resolution detectors in coincidence. Images of the radionuclide activity distributions obtained after reconstruction, are presented. The performance of the detectors is discussed and the analysis of the experimental results is assessed by computer simulations.

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Recent Progress in 2D-ACAR in Metals and Alloys in Bristol

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This talk is intended to provide a brief guide to positron annihilation as a means of study of electronic structure of metallic systems. It would start with an outline of the technique including extraction of information with an emphasis on the Fermi surface. We shall then give an account of recent work on aspects of Fermi surface related materials properties in novel and some complex systems.

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Positron Annihilation with Admixture Electrons in Some Nickel Alloys

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The measurements of cold rolled nickel alloys with 1 at.% of Ti, Zn, Ge, Zr, In, Sb and Pb by positron lifetime and two-detector Doppler broadening techniques have been done. The cold-rolled samples submitted to long lasting tempering at about 800 K followed by slow cooling to the room temperature were measured by positron lifetime and two-detector Doppler broadening techniques again. The annihilation measurements of the admixture materials (Ge, Sb - monocrystals), (Ti, Zn, Zr, In, and Pb - polycrystals) and matrix - (Ni - polycrystal) have been done, too.

The analysis of the annihilation characteristics for defected and well annealed samples shows that the probability of annihilation of positrons with admixture (impurity) electrons for the cold rolled samples is higher than that for well annealed samples. The differences in probabilities are evidence of numerous defect-impurity states presented in deformed samples.

The comparison of possibilities of the Doppler broadening technique and the positron lifetime technique in the field of detection of defect-impurity states will also be discussed in the paper.

Investigation of Electron-Positron Correlations by Monte-Carlo Simulation

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Earlier studies, as well as recent calculations of positron annihilation rates in metals, show that some basic problems concerning electron-positron (e-p) interaction have not been solved satisfactorily, even for homogeneous media. This work is devoted to the "computer experiment", i.e. the investigation of the above interactions is made by Monte Carlo (MC) simulation. It is evident that the starting point should be the positron in electron gas. Comparing with the previous works on the subject the considerable progress has been achieved. Firstly, the method of "exact determining" of positron annihilation rates on the basis of variational trial function has been worked out. Moreover, one has found the way of calculating the enhancement factors, the quantities not achievable within the MC method since now. The annihilation rates obtained by other authors using MC have the wrong tendency, they fall down below $2 \cdot 10^9 s^{-1}$ for $r_s > 4$. Since Lantto's results (exploited in commonly used Boroński-Nieminen and Puska formulas) were based on the same assumptions concerning the variational wavefunction, this behaviour of the rates calls his calculation in question.

These rates have been corrected in this work for the metallic range of r_s by the appropriate construction of the trial function. The 3-particle correlations (i.e. dependence of the electron-electron (e-e) interaction on the distance from the positron) have been taken into account. Besides, the dependence of the e-p interaction on the electron state has been explicitly introduced to the Slater determinant. Adding a possibility of Friedel-type oscillations into the Jastrow e-e and e-p factors resulted in diminishing the total energy of the system by 11%.

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Slow Positron Implantation Spectroscopy – a Tool to Characterize Vacancy-Type Damage in Ion-Implanted 6H-SiC

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Positron Annihilation Spectroscopy (PAS), mainly in the form of **S**low **P**ositron **I**mplantation **S**pectroscopy (SPIS), is used to study vacancy-type damage in ion implanted SiC. Thereby, the generation and use of monoenergetic positrons is essential as they serve as the tool to investigate depth dependant defect profiles caused by ion implantation. Physical information is derivable from the Doppler broadened annihilation lineshape, e.g. via the definition of characteristic lineshape parameters.

Basic physics behind the method will be explained and the derivation of a defect profile will be exemplified. Finally, several results on ion implanted SiC are presented. It is generally found that the vacancy-type damage formed is a function of substrate temperature during implantation and post-implantation annealing. In addition, a strong influence of the sequence of implantations on the vacancy-type damage formed is shown.

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Porosity of Low-k Materials Studied with Use of Positrons

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As pointed out in the *Interconnection* chapter of the 2003 *International Technology Roadmap for Semiconductors* [1] one of the most difficult challenges to reach the near term technology node of ≥ 45 nm / through 2009 is the realization and integration of very low dielectric constant materials ($\kappa < 2.1$). At present some low κ materials with κ values around 2.9 have just been introduced in the production of electronic devices.

In this lecture we shall review the information about porosity in low κ materials obtainable with Depth Profiling with Positron Annihilation Spectroscopy (DP-PAS): positron annihilation lifetime spectroscopy (PALS), Doppler broadening spectroscopy (DBS) and 2-3 gammas ratio of positronium (3γ-PAS). A brief comparison will be done with other techniques used in the characterization of low- κ films: small angle neutron scattering (SANS) and small angle x-ray scattering (SAXS) used in combination with x-ray reflectivity (XRR), ellipsometric porosimetry (EP).

In particular DP-PAS measurements on SiOCH type low κ films will be presented. SiOCH films have been studied as a function of thermal treatments, gas permeation, and different condition of deposition. The films have been also characterized by vibrational spectroscopy and the composition measured by nuclear techniques.

[1] *International Technology Roadmap for Semiconductors* (2003).

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Primary Chemical Reactions Induced by Transformation of Radioactive Nuclei in Solids at Low Temperatures. Investigation by Means of the Emission Mössbauer and Positron Spectroscopies

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Numerous measurements of the yields of final products ($^{57}Fe^{2+}$, $^{119}Sn^{2+}$) of transformation of the "Mössbauer" nuclei (^{57}Co, ^{119}Sn) in various frozen glassy and crystalline polar and nonpolar media have been done and compared with the Ps formation probabilities in analogous conditions. Similarity between chemical transformations occurring in positron tracks and in the vicinity of the "Mössbauer" atoms after Auger electron emission has been revealed. It becomes apparent in similar variations of the final products vs concentration of electron scavengers, temperature, degree of crystallinity. Such a behavior is due to participation of presolvated electrons in the primary chemical reactions in positron tracks as well as in nanovicinities of radioactive atoms.

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Relaxation of Free Volume in Polycarbonate and Polystyrene Studied by Positron Annihilation Lifetime Spectroscopy

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In the present talk, we present the time evolution of polycarbonate (PC) and polystyrene (PS) free volume, which occurs after thermal rejuvenation above the glass transition temperature (T_g). In addition, PC and PS free volume is studied after plastic deformation by means of cold rolling, which is believed to reinitiate physical aging similarly to thermal rejuvenation. For this reason this process is known as "mechanical rejuvenation". We employed positron annihilation lifetime spectroscopy (PALS) to characterise the free volume properties of PC and PS. The value of the long lifetime component that is attributed to the decay of ortho-positronium ($\tau_{o\text{-}Ps}$) and its intensity ($I_{o\text{-}Ps}$) are used to characterise respectively the size and the concentration of the free volume holes.

Contrarily to the common interpretation that application of large stresses in the glassy state can erase the thermo-mechanical history of the sample, our results suggest that the effect of plastic deformation on the polymer microstructure is far different from that of a thermally rejuvenated sample. In particular, plastic deformation results in an increase of $\tau_{o\text{-}Ps}$ and a decrease of $I_{o\text{-}Ps}$, whereas rejuvenation above T_g results in an increase of $I_{o\text{-}Ps}$ while $\tau_{o\text{-}Ps}$ remains unchanged. In addition, physical aging below T_g after plastic deformation manifests as a reduction of $\tau_{o\text{-}Ps}$, whereas a decrease of $I_{o\text{-}Ps}$ is observed after thermal rejuvenation. The ability of PALS to characterise the free volume as a combination of hole size and hole concentration corroborates the idea of an amorphous-amorphous transition, rather than that of a "mechanical rejuvenation" as proposed in the past to explain the ability of plastic deformation to reinitiate physical aging.

Thermal Defects in Iron-Based Solid Solutions

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Thermal equilibrium studies with positron annihilation spectroscopy show that an increase in the temperature of a metal goes together with prolonging of the positron lifetime in the material. This can be explained as a result of two processes - thermal expansion of the crystalline lattice and creation of vacancies in the lattice. The latter is observed for iron crystal when its temperature is higher than about 1070 K. Simultaneously, for the temperatures not exceeding 1070 K, the positron lifetime τ_p in iron increases with temperature at the rate α_p about three times larger than one could expect having known that in the first approximation τ_p is proportional to the reciprocal of the "free" electron density, determined by thermal expansion of the crystalline lattice. The unexpected large value of α_p speaks in favour of the suggestion that an increase in the temperature of iron is accompanied by creation of some low-electron-density regions that attract positrons and prolong their lifetime. It seems that the regions arise due to thermal distortions (dilatations) of the crystalline lattice leading only to a transient increase of the distance between a certain number of neighbouring atoms and not resulting in creation of a stable vacancy. This so-called prevacancy effect was observed for the first time on In, Cd and Zn in the early 1960's but its intensively studies began in the middle of 1970's and lasted for approximately two decades.

For a long time the positron annihilation findings concerning the "low-temperature" distortions of the metal lattice could not be verified by another method due to lack of it. Only in recent years it appeared that such distortions in the crystalline lattice of binary, iron-based solid solutions can be observed also with the ^{57}Fe Mössbauer spectroscopy [1-3]. The latter suggests that occurrence of the prevacancy effect in metals is not connected with a special behaviour of positrons in the materials.

[1] J. Chojcan, *J. Alloys Compd*. **337**, 25 (2002).
[2] J. Chojcan, *Acta Phys. Polon. A* **100**, 723 (2001).
[3] J. Chojcan, *J. Alloys Compd*. **373**, 33 (2004).

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Defect Study on Deformed Fe-Si Alloys with Positron Annihilation Techniques

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Fe-Si alloys possess a combination of low magnetostriction with high saturation magnetization, which make these materials especially suitable for the construction of transformers. Despite the improvement of the magnetic properties with increasing Si content, the content of this element is limited to about 3.5 wt% in the commercial products. This limit is due to the drastic reduction in ductility for compositions above 4.5 wt% which causes problems in the rolling process used in sheet production. Interest in the improvement of these commercial products has resulted in great efforts towards the development of new processing routes to the production of Fe-Si alloys with 5.5–6.0 wt%. Besides the Si content, the magnetic properties such as coercive force, saturation magnetization and power loss are strongly influenced by the structural state, grain size and defect density.

A set of Fe-Si samples with different Si content, varying from 0 to 7.6 wt%, was investigated. Different deformations were performed on these samples so measurements can be done to investigate the defects in the alloys. An exponential decay of the S-parameter in function of the time can be observed after deformation of the samples. The decay constant increases with increasing Si content. During the measurements of the samples with increasing Si content, the initiation of DO_3 structures can be seen above 6 wt% of Si, as well as the decoration by impurities. The Doppler broadening annihilation spectroscopy was used. The results will be presented.

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Defects in Ultra-Fine Grained Mg and Mg-Based Alloys Prepared by High Pressure Torsion Studied by Positron Annihilation

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Despite the favourable strength and thermal stability, a disadvantage of the Mg-based alloys consists in a low ductility. Recently it has been demonstrated that ultra fine grained (UFG) metals with grain size around 100 nm can be produced by high pressure torsion (HPT). A number of UFG metals exhibit favourable mechanical properties consisting in a combination of a very high strength and a significant ductility. For this reason, it is highly interesting to examine microstructure and physical properties of UFG Mg-based light alloys. Following this purpose, microstructure investigations and defect studies of UFG Mg and selected UFG Mg-based alloys prepared by HPT were performed in the present work using positron annihilation spectroscopy (PAS) combined with X-ray diffraction (XRD), microhardness measurements, and direct observations of microstructure by TEM.

Positrons are trapped at dislocations in Mg and Mg-alloys deformed by HPT. Number of dislocations increases with the radial distance r from the center to the margin of the sample most probably due to an increase of strain with r. No microvoids (small vacancy clusters) were detected. Mg-alloys deformed by HPT exhibit homogeneous UFG structure with grain size around 100 nm and high dislocations density except Mg-15Gd alloy, where UFG structure was not formed. On the other hand, pure Mg deformed by HPT exhibits a binomial type of structure which consists of “deformed regions” with UFG structure and a high dislocation density and dislocation-free “recovered regions” with large grains. It indicates a dynamic recovery of microstructure during HPT processing.

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Positron Annihilation Spectroscopy of Ultra Fine-Grained Metals Prepared by Severe Plastic Deformation

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Ultra fine-grained (UFG) metals with a mean grain size of several hundreds of nanometers are nowadays considered to be promising materials for various industrial applications. This is due to their improved mechanical properties compared to traditional polycrystalline metals. Obviously, a complex structural investigation at the nanoscale level is valuable for an understanding of the formation of the UFG structures and their thermal stability.

Recent investigations of UFG metals (Cu, Fe, Ni, Mg, Mg-Gd) performed within a Prague-Rossendorf-Ufa collaboration will be rewieved. The specimens were prepared by severe plastic deformation: the high-pressure torsion and equal channel angular pressing. Positron annihilation spectroscopy was used as the main method including (i) the conventional lifetime and coincidence Doppler broadening (DB) measurements with ^{22}Na and (ii) the slow-positron implantation spectroscopy (SPIS) with DB measurement. Other methods were also involved: TEM, XRD and microhardness. First, the mean grain size was determined and defects were identified in the *as-deformed* materials. Defects concentration and spatial distribution were studied in details. Dislocations situated in distorted regions along grain boundaries, and a few-vacancy clusters distributed homogeneously inside dislocations-free grains, were observed in the UFG Cu, Fe and Ni. On the contrary, uniform spatial distribution of dislocations and no microvoids were found in the Mg-based alloys. Subsequently, the thermal evolution of the UFG structures during isochronal annealing was studied.

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Outdoor Ageing of an Ethylene-Propylene Copolymer: a Positron Annihilation Study

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An investigation on the environmental degradation of an ethylene-propylene copolymer has been carried out through positron annihilation lifetime spectroscopy, density and differential scanning calorimetry measurements. Polymer sheets were exposed to sunlight up to 11000 hours. Density and melting enthalpy increase with ageing, while ortho-positronium (o-Ps) intensity decreases; concerning o-Ps lifetime, it does not show significant variations up to 4400 hours. At higher exposures it starts to decrease.

The experimental results imply that outdoor ageing produces an increased crystallinity of the copolymer; also a degradation is likely to occur, with possible formation of carbonyl groups. The corresponding Ps inhibition is one of the reasons for the decrease of o-Ps intensity, the other one being the reduced amount of the amorphous phase available. The behaviour of o-Ps lifetime seems to exclude chemical quenching of Ps from carbonyl groups; in fact, the decrease observed at the highest exposures can be interpreted in terms of a shrinking of the nanoholes trapping Ps.

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Doppler Broadening Positron Annihilation Technique for Investigation of the Thermo-Shrunken Polyethylene

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A Doppler broadening positron annihilation technique was used to investigate temperature changes of the parameters of the 511 keV annihilation line emerging from thermo-shrunken polyethylene. Three different kinds of polyethylene samples were chosen for measurements. All of them were made of commercially available polyethylene. All of the measurements were performed in vacuum. Comparison of the parameters of the annihilation line observed in the investigated polymer is presented.

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Investigation of the Temperature Dependence of Free Volume in Polymethylpentene by Positron Annihilation Method

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Positron lifetime measurements in polymethylpentene were performed in a wide temperature range. A conventional fast-slow coincidence lifetime spectrometer with plastic scintillators was used. All the measurements were made in vacuum. Additional measurements (X-ray diffraction, differential scanning calorimetry and mechanical spectroscopy) were also performed to establish properties of samples. Mean free volume radii and fractional free volume in the investigated samples were estimated from the positron lifetime measurements results.

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Experimental Verification of the Blob Model for the Formation of Ps

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The blob model for the formation of positronium was proposed by Stepanov and Byakov. Although it could be considered as an extension of the spur model, it offers many extra possibilities and is more sound from the radiation chemistry point of view. However, a proper coding of this model leads to non-exponential lifetime spectra, and standard multi-component analysis is no longer adequate for materials such as polymers. In polymers there are still many unsolved questions, such as 1) What is the meaning of I_3 , 2) Why is $I_1 > I_3/3$ and 3) Why is $\tau_1 >> 124$ ps ? Other questions concern the possible delayed formation of positronium.

Age Momentum Correlation (AMOC) experiments were performed on linear and on crosslinked PMMA at different temperatures and were analysed with the non-exponential blob model. We show that the three problems mentioned before are easily solved and the blob model also gives an alternative explanation for the well known young-age broadening in materials, which form Ps. We will also show that standard multi-exponential analysis leads to erroneous results for the values and intensities of the shorter lived contributions.

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The Influence of the Defect Structure on the Nitriding of Fe by PIII

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The wear resistance of iron alloys can be substantially improved by nitriding using several techniques. One promising technique is Plasma Ion Immersion Implantation (PIII). A case study for the characterization of the PIII nitriding of iron alloys is the PIII nitriding of pure Fe. In this study the influence of the defect structure of Fe prior to the PIII treatment is investigated.

Fe samples of 99.98% purity and with a different defect structure were PIII treated at different temperatures. A first set of samples was kept in the annealed state, a second set was polished and a third set of samples was chemically etched in order to remove the defects introduced by the polish. The samples were PIII treated at 300°C, 400°C and 500°C. Depth profiling of the samples was achieved using positron annihilation spectroscopy with a slow positron beam, FIB/SEM and nanoindentation. These results will be discussed in accordance to the presence of the different Fe phases detected by Mössbauer analysis and the N depth distribution measured by RBS.

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To Mix or Not to Mix? Positive Mixing Volume in PA/P(n-BA-co-MMA) Blends

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In blends PA/P(n-BA-co-MMA) the positive mixing volume was found accompanied by not additivity of free volume [1]. The blends are not miscible, two-component systems where acrylic rubber is dispersed in a glassy matrix of polyamide 6. The properties of the blends were studied with use of many techniques [1]. Their compatibility was revealed by improvement of the notch impact strength in comparison to the unmodified polyamide. The formation of a graft or block copolymer as a result of reaction in situ between the polyamide and the acrylic rubber was suggested, which was supported next by the infrared spectroscopy [2]. The positive volume of mixing for the blends is, in case of non miscible polymers, assumed as an evidence of looser packing of macromolecular chains in separate phases and formation of the additional free volume at the phase boundaries [3].

In the paper the influence of crystallinity of polyamide is studied. Experimental results of PALS,WAXS, SAXS, infrared spectroscopy and DSC measurements for polyamide 6, submitted to the action of I_2, hot water and liquid nitrogen, will be given. The action of the agents results in different morphology of the studied samples of polyamide [4]. In a model the diffusion of positronium between two neighbouring layers (a crystalline lamella and an amorphous one) is studied. The results suggest that o-Ps atoms, if formed in crystalline lamellae, diffuse out from there to amorphous regions.

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Density and Size Distribution of Holes from PALS and PVT Experiments: the Temperature and Pressure Dependence of the Free Volume in Fluoro Polymers

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We present the temperature (100 - 473 K, 0 MPa) and pressure (0.1 - 448 MPa, 22.5 °C) dependency of the free volume hole size distribution (mean value $<v_h>$ and dispersion σ_h) in the fluoroelastomer PFE obtained from a LT9.0 analysis of PALS data. We show that for a correct lifetime analysis the dispersion in both the positron (τ_2) and o-Ps lifetime (τ_3) must be taken into account. Moreover, the mean hole volume $<v_h>$ should be calculated as mean of the hole size distribution and not directly from the (mean) τ_3. Indications were found that o-Ps may prefer larger holes with a weight approximately given by the hole volume v_h. The hole size distribution is discussed in terms of the theory of thermal volume fluctuations.

Employing the Simha-Somcynsky equation of state the excess free (hole) volume fraction h and the specific free and occupied volumes, $V_f = hV$ and $V_{occ} = (1 - h)V$, were estimated from the specific total volume V. From a comparison of $<v_h>$ with V_f the specific hole number N_h' was estimated. N_h' was determined to be constant and the same in compression and thermal expansion experiments. We found that the occupied volume V_{occ} exhibits a remarkable compressibility, while it shows (for $T > T_g$) almost no thermal expansion. When taking this into account the discrepancy in V vs. $<v_h>$ plots between compression and thermal expansion experiments discussed in the literature disappears. The free volume structure of the rigid amorphous fraction in semicrystalline PTFE as detected by PALS and PVT is discussed.

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The Temperature Dependence of the Free Volume in Poly(Dimethyl Siloxane) (PDMS) from PALS and PVT Experiments

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We present DSC (123 - 323 K), PVT (300 - 430 K, 0.1 - 200 MPa), and PALS (100 - 473 K, 0 MPa) studies of the structure and free volume in a 35 wt. % filled and an unfilled, semicrystalline poly(dimethyl siloxane) (PDMS). We analysed the lifetime spectra employing the routine LT9.0 and allowing a dispersion (standard deviation σ_i) in all of the three lifetimes: τ_1 (p-Ps), τ_2 (e^+), and τ_3 (o-Ps). We found that correct parameters of p-Ps annihilation (τ_1 = 115(±3)ps, I_1/I_3 = 0.32(±0.03), σ_1 = 0 - 20 ps) are obtained only by allowing a dispersion in τ_2 and τ_3, otherwise $I_1/I_3 > 1/3$. The dispersion in τ_2 and τ_3 comes from the size and shape distribution of free volume holes where e^+ and Ps annihilate. When heating from 100 to 473 K the o-Ps parameters τ_3 and σ_3 and the e^+ parameters τ_2 and σ_2 show changes due to glass transition (165 K) and melting of crystals (235 K) formed at lower temperatures. The o-Ps intensity I_3 exhibits changes due to cold crystallisation above a temperature of ~165 K and due to melting at 235 K. These transitions are confirmed by the DSC studies. Surprisingly, only I_3, but not τ_3, is affected by the filler. Employing the Simha-Somcynsky equation of state the excess free (hole) volume fraction h and the specific free and occupied volumes, $V_f = hV$ and $V_{occ} = (1 - h)V$, were estimated from the specific total volume V (see ref. [1]). From a comparison of the mean hole volume $\langle v_h \rangle$ with V_f (see ref. [2]) the specific hole number N_h' was determined to be constant. We found that the occupied volume V_{occ} exhibits a remarkable compressibility, while it shows almost no thermal expansion.

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Positron Lifetime Measurements of Subsurface Region in Aluminium Alloy and Aluminium Alloy Composite after Dry Sliding

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Discontinuously reinforced light metal matrix composites (MMCs) constituted of high–strength metallic alloys reinforced with ceramic particulates or whiskers are widely employed in aerospace and automotive industries due to their reasonable mechanical properties. Although the wear of metal matrix composites is a very complex process, aluminium alloy based composites exhibits often better wear resistance in comparison to the unreinforced alloys.

The samples of the aluminium alloy AK12 and aluminium alloy composite AK12 with aluminium oxide particles were exposed to the sliding against the steel in the pine-on-disc machine. After that the defect depth profile was measured using positron lifetime spectrometer. The well visible defects depth profile detected in the AK 12 alloy extended up to 300 μm but for the composite AK12 the range of this profile was significantly shortened to the value less than 100 μm. The subsurface zones have been also examined using scanning electron microscopy. We intend as well to compare the results with those obtained for other aluminium alloys: PA6 and PA38, in order to show that the defect profile induced during friction treatment depends in the significant way on the alloy composition.

Near Surface Distribution of Defects Using Positron Implantation Profile - a New Experimental Method

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We intend to present the new experimental setup, which allows us to trace the positron implantation profile in the matter. The value of the linear absorption coefficient, or mean penetration depth of positrons emitted from ^{22}Na isotope in different materials has been measured using this setup. Nevertheless, we used it as well for measurement, in a nondestructive way a defect depth profile in light metals and alloys. We demonstrated it for the pure aluminium sample whose surface was damaged in the blasting treatment. A well defined defect profile was detected which coincides well with that established using another technique. The presented setup can be useful for detection of the subsurface zones for instance in tribological studies.

Many-Body Theory of Positron Annihilation Gamma-Ray Spectra

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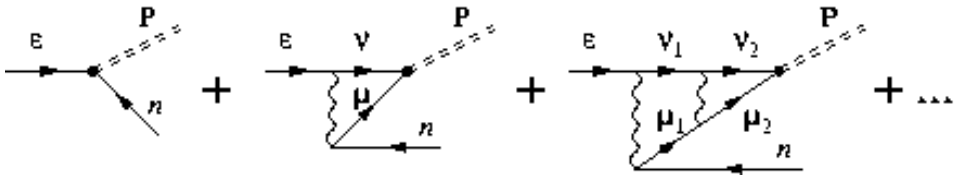
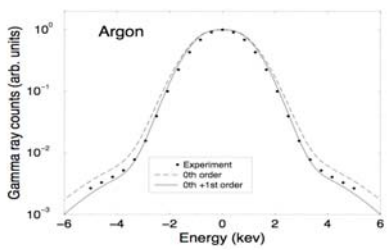
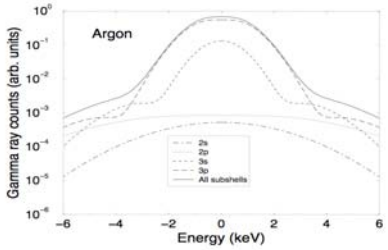
Positron-matter interactions have been studied extensively and currently theory is being developed to support experimental observations [1]. As the motion of many electrons and the positron is correlated, we propose to study this using many-body theory. Many-body theory describes electron-positron correlation using diagrams instead of multiparticle wavefunctions. The amplitude of the emission of two gamma-quanta with the total momentum **P** is:



ε is the incident positron, *n* is the hole, ν and μ are intermediate positron and electron states, wavy lines represent Coulomb interactions, and double dashed lines describe gamma quanta.

The first two diagrams lead to the following results for the spectra, where the energy is measured from the centre of 511 keV peak.





The inclusion of the 1st order correlation correction improves the agreement with experiment [2], for Helium, Neon, Argon, Krypton and Xenon. It also doubles the total annihilation rate, which indicated that higher-order terms must be included.

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Defects in Neutron Irradiated Copper Investigated by Positron Annihilation Spectroscopy

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Neutron irradiated copper has been the subject of a number of investigations by Positron Annihilation Spectroscopy (PAS). The present talk will concentrate on the information that has been obtained by PAS about the defect microstucture in copper after neutron irradiation, including the effects of irradiation temperature and annealing temperature. Quantitative comparison will be made with data from Transmission Electron Microscopy (TEM) and we will discuss to which extent the two techniques give overlapping or supplementary information. The question whether PAS is able to detect Stacking Fault Tetrahedra (SFTs), which are clearly observed by TEM, will be dealt with in some detail.

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Application of Positron-Annihilation-Induced Auger Electron Spectroscopy to the Nanoparticle Coverage

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Recent studies of the sputtered surface of an annealed Fe-1.0 wt % Cu (2h aging) alloy using Positron-annihilation-induced Auger Electron Spectroscopy (PAES) reveal that positron annihilation with Cu core electrons takes place at about 5 times the nominal concentration level in the alloy. PAES measurements made on the Fe-Cu alloy surfaces whose Cu concentration has been enriched by additional annealing show a large enhancement in the annihilation rate with Cu core electrons relative to its surface concentration as measured by EAES. The observed large enhancement of the Cu PAES signal for the vacuum annealed surfaces is similar to that seen for the PAES signal of Au deposited on Cu [1].

The results of PAES studies of sputtered surfaces of the Fe-Cu alloy with quantum-dot like Cu nanoparticles embedded in Fe and submonolayer films of Au and Pd deposited on Cu(100) are analyzed by performing calculations of positron surface states and annihilation characteristics. Estimates of the positron binding energy, work function and annihilation characteristics performed for studied surfaces reveal their strong sensitivity to nanoparticle coverage. Trapping of positrons at nanoparticles on studied surfaces is determined from calculated positron surface state wave functions. Theoretical core annihilation probabilities are compared with experimental ones estimated from the measured Auger peak intensities.

Research supported in part by the National Science Foundation and the Robert A. Welch Foundation.

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Defects Associated with Nanostructures in AlZnMg and AlCu(Mg) Alloys

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Knowledge of atomic mechanisms leading to the formation of nanoprecipitates during the decomposition of supersaturated solid solutions is at the basis of the current effort to improve age-hardening effects in light alloys. To this end, a combination of experimental techniques (three dimensional atom probe field ion microscopy, high-resolution electron microscopy, microhardness, positron annihilation spectroscopy and small-angle X-ray scattering) has been used to observe various aspects of precipitation phenomena in AlZnMg, AlCu and AlCuMg alloys. The present work is focalised to positron annihilation spectroscopy studies addressed to the kinetic and chemical characterisation of solute aggregates containing open volumes (vacancies and/or misfit regions at precipitate-matrix interfaces). Lifetime spectroscopy (LS) and coincidence Doppler broadening spectroscopy (CDB) were adopted. Both techniques are sensitive to the chemical environment of open volumes defects in age-hardening alloys. The difference is that LS is mostly sensitive to the electron density inside open volumes, while CDB enables to detect Zn or Cu on the walls of open volumes. The information presented can be summarised as follows.

1. Study of the secondary ageing at low temperature, after few minutes of artificial ageing. The increase of the positron lifetime and the concomitant recovery of the Zn or Cu signal in CDB spectra clearly show that the residual solute supersaturation leads to the formation of coherent Zn-Mg-v or Cu-Mg-v.
2. Differentiation of the age-hardening during artificial ageing between the AlZnMg and AlCu(Mg) alloy systems. In AlZnMg alloys hardening is concomitant with the loss of coherency, on the contrary AlCu(Mg) alloys is associated with coherent structures.

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Positron Induced Ion Desorption

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The determination of structure and electronic property of adsorbed molecules on a surface is one of the most important subjects in surface science. Positrons have great potential as a tool for surface analysis because they have negative or very small work functions for many substances and they could have surface states. Ionization of absorbed molecules by positrons could be a powerful tool for detection of molecular ions. In this study, ion desorption excited by positrons has been investigated using an electrostatic beam.

An electrostatic positron beam for ion desorption experiment has been developed. Positron energy was fixed at 2 keV and they were transported with 5 sets of Einzel lenses and 2 sets of deflectors over 1.2 m distance up to the sample chamber. About 4,000 positrons/s were obtained at the sample position with a beam diameter of 2.5 mm FWHM. A quadrupole mass spectrometer (Q-mass) was used for detection of desorbed ions and placed at 60° with the positron beam axis. The samples used were Au surfaces covered with alkanethiols. It is well-known that self-assembled monolayer can be formed by immersing Au substrate to alkanechiols or organic disulfides solutions, and that the bonding is formed between Au and S atoms of thiol molecules in alkanethiol/Au systems. Ethanethiol/Au and pentanethiol/Au were prepared by immersing in 5 mM alkanethiol solution of ethanol for more than 6 hours.

Figures 1 shows a mass spectrum obtained when 2 keV positrons were injected to ethanethiol/Au. A peak due to molecular ions, or $C_2H_5S^+$ ions, clearly appears around M/z of 61 and no fragmented ions are observed. In pentanethiol/Au sample, a peak at M/z of 103 is seen and it is attributed to $CH_3(CH_2)_4S^+$. Thus, ion desorption induced by positrons can be observed for the first time with the identification of ion species. It is considered that positrons, which diffuse back to the surface, annihilate the bonding electrons between S and Au. It is not, however, concluded whether this annihilation is a direct process or via positronium formation. In order to clarify the exact mechanism of desorption and to utilize this phenomena as a tool for surface science, further investigations such as measurement of energy distribution of the desorbed ions and quantitative estimation of the desorption cross section are needed.

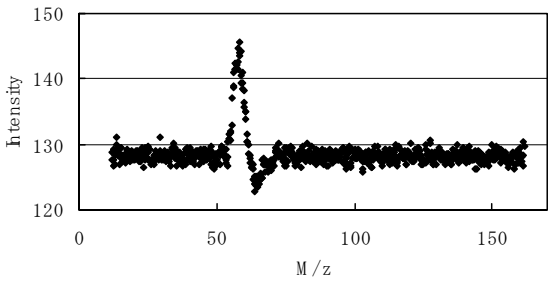

Fig. 1 Mass spectrum obtained when 2 keV positrons are injected to ethanethiol/Au. Beam intensity is about 4,000 /s.

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Positron Annihilation and CPM Measurements on a-Si:H – a Comparative Approach

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Thin films of hydrogenated amorphous silicon (a-Si:H) have been deposited on crystalline silicon substrates by Plasma Enhanced Chemical Vapour Deposition – PECVD at *rf* power densities, P_D, ranging from 3.6 to 28.6 mW/cm^3 and deposition temperature, T_{subst}, ranging from 200 to 300ºC. A positron beam was used to analyse the influence of these deposition parameters on the film defect structure and Constant Photocurrent Method (CPM) was used to measure the density of deep states inside the band gap (DOS) of the semiconductor films.

The Doppler parameters, S_{film} and W_{film}, were obtained from the fit to the *S*(E) and *W*(E) data as function of positron energy for each film using VEPFIT [1]. The linear behaviour of the points (S_{film},W_{film}) characteristics of each film in the (*S*,*W*) plot is strongly indicative that positron annihilation takes place on two different type of defects. Those defects can be related to small vacancy type defects, probably divacancies, and large vacancy clusters like microvoids.

For each deposition temperature the S_{film} parameter increases initially with P_D and reaches its maximum at a relatively low P_D (~7.3 mW/cm^3) value, then decreases continuously up to $P_D \cong 21.7$ mW/cm^3. This can be associated with the presence of both defect types in different relative concentrations. Moreover, for this P_D range the CPM measurements reveal no strong variation on the density of deep defects. Solar cells were made using films prepared within the same P_D range. The evolution of the optoelectronic characteristics of these solar cells is quite similar to the observed on the S_{film} parameter. In this work we intend to discuss the implications of the results by CPM and by positron annihilation measurements.

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Pressure Effects in *ortho*-Positronium Annihilation

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Up to now not too many papers devoted to the influence of pressure on positronium formation and decay were published. Similarly as in the case of temperature dependences, one can expect many interesting effects. In this paper some of them are described.

1. Squeezing out the energy level in the potential well, in which Ps is trapped. There is a minimal void radius at which the energy level for a particle in the well can exist; reduction of the void size under high pressure can lead to the disappearance of the energy level and therefore to the disappearance of positronium. This effect was demonstrated in the case of biphenyl and naphthalene. In both these solids Ps formation can be eliminated also by lowering the temperature, i.e. free volume is created by thermal motions.

Small free volumes can be formed in mixed crystals, in the vicinity of small guest molecules. In p-terphenyl doped with 0.6% of anthracene the o-Ps component diminishes its intensity and lifetime with pressure, but is still present even at 1.3 GPa. The form of temperature and pressure dependences is essentially different.

2. Pressure induced phase transitions, like from rotator to rigid phase in solid *n*-alkanes. In this case $\partial T_{tr}/\partial p > 0$ and the increase of pressure is equivalent to lowering the temperature. In *n*-nonadecane at 302 K (3 K below the melting point) the transition occurs already at the pressure of 32 MPa. When the pressure is produced by gaseous medium (e.g. argon) the intercalation of gas to the gap between the molecular lamellae and to the big volume defects modifies the $\tau_3(p)$ dependence. In p-terphenyl the phase transition at 193 K has negative $\partial T_{tr}/\partial p$ value, thus it cannot be observed under pressure.

3. The rise of I_3 intensity with time, observed in alkanes after the transition from rotator to rigid phase by lowering the temperature, is not seen when the transition is induced by the pressure; on contrary, the intensity diminishes with the time constant of several hours.

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Imaging of Deformation Zones by Scanning Positron Microscopy

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Defect imaging in the micron range is an important step towards an understanding of the microscopic processes of fatigue and fracture. The Bonn Positron Microprobe (BPM), employing a fine-focus positron beam, is now looking back on seven years of operation. An overview of our recent works on defect imaging of deformed materials is given and the different fields of interest in our research are presented. This will include:

- Imaging of the plastic zones in front of fatigue cracks.
- Analysis of the influence of cutting parameters on the subsurface damage in high speed cutting.
- Aging effect in industrially used aluminium alloys AA 2024 and AA 6013.

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Magnetic Induced Diffusion of Positrons in Metals

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The effect of a magnetic field on the positron diffusion is studied, using a superconducting solenoid, which provides a magnetic field up to 5 Tesla. Slightly deformed Copper is used as sample material.

The measurement was made at different temperatures. A decrease of the S-parameter with rising magnetic field is. The slope of the S-Parameter can be explained by a numerical diffusion model which will be presented.

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Positronium Formation at Low Temperatures in Polymers and Other Molecular Solids

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Positronium(Ps) formation mechanism by shallowly localized long-lived electrons and positrons at low temperatures explained successfully the Ps formation enhancement at low temperatures observed in polymers and other molecular solids. The expected phenomena by this Ps formation mechanism, such as an effect by visible light exposure and delayed Ps formation, were observed.

Now, positron annihilation methods can be tools to investigate the shallowly localized electrons, such as trapped electrons or anions. There are some other methods to detect these electrons, such as electron paramagnetic resonance (EPR), light absorption. There are some advantages of use of positron methods to see these electrons.

Some possibilities of application of this new Ps formation, such as a new idea of observing spin polarized positrons by this Ps formation, will be also introduced. Ps formation by spur process will not be affected by positron spin direction, because the spins of excess electrons in the positron spur are randomly distributed. However, the shallowly localized long-lived electrons can be polarized when they are placed in magnetic field at very low temperatures. It is probably possible to see the polarity of positrons by the Ps formation with these polarized electrons.

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Variable-Energy Positron Annihilation as Highly Sensitive Nanoporosimetry for Porous Low-*k* Films*

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Positron annihilation (PA) has been applied to measuring critical pore sizes in various materials, including polymers, porous oxides, and other systems [1]. There are several advantages of PA over other methods; it is nondestructive, sensitive to holes of 0.3-50 nm in size and can detect buried, isolated pores that are not accessible to conventional probes. In recent years, PA with a variable-energy positron beam has emerged as a powerful tool for the investigation of porous thin films (from tens nm up to several μm in thickness) that are promising to be used as low-*k* dielectric insulating materials in the semiconductor industry [2-6]. This talk concerns the thin film pore characterization, accomplished by three different techniques in PA. The target films were four kinds of hydrogen-silsesquioxane films, prepared by spincoating of precursor solutions containing various concentrations of sacrificial porogen on a silicon wafer.

1) Positron annihilation 3γ-ray measurements. A part of energetic positrons implanted into films form into *ortho*-positronium (*o*-Ps) atoms. In the presence of open pores, they can diffuse out from the film into vacuum and annihilate into 3γ-rays with an intrinsic lifetime of 142 ns. Hence the positron 3γ decay probability ($I_{3\gamma}$) is related to the film open porosity [3,5]. It was found that $I_{3\gamma}$ for the as-deposited films increases with increasing porogen concentration, and is reduced dramatically with capping by nonporous silica on the film surface. These results clearly show that the film prepared with the porogen has an open porosity which increases with increasing porogen concentration [4]. The high open porosity was also confirmed by positronium time-of-flight measurements; an increased amount of the energetic Ps emitted from the film surface was observed for the film with the highest open porosity [7].

2) Positron annihilation lifetime measurements. The pore dimensions of capped films were deduced from *o*-Ps lifetimes using an available model for nano-sized pores [1]. The calculated pore radii for films prepared with the porogen were in the range from about 1.1 nm to 2.6 nm, while the pore radius of the film prepared without porogen was about 0.5 nm. The pores were found to be enlarged with increasing porogen concentration and film open porosity [4]. These results signify that the pore size can be controlled by the porogen method.

Results of nano-clustering silica low-*k* films will also be presented.

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Crystallization Process in Porous and Nonporous Vycor Glass

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Crystallization of silica in Vycor glass was observed using PALS and X-ray diffraction methods. Three-component glass of Vycor type, composed of sodium, boron and silicon oxides was treated in different ways in order to obtain various pore radii in the material.

Three kinds of glass were investigated. First one, nonporous Vycor glass was heated at 600, 625, 650 and 675^0 C in periods of time changing from 0.5 to 48 h to obtain various crystallinity degree of silica. Such a crystallinity degree found from X-ray data correlates very well with o-Ps intensity decrease determined from PALS.

Second kind of investigated material was glass containing narrow pores of radii from 1 to 2 nm produced by liquation at various thermal conditions and etching in acid. Two o-Ps components found from PALS were compared with X-ray diffraction data.

Third stage of investigations concerned porous glass containing mesopores, and reheated at temperatures 710, 725 or 740^0C and time changing from 8 to 168 h (7 days) to recrystallize silica.

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Three-Quantum Annihilation in Porous Vycor Glass

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Extension of the Tao-Eldrup model toward large free volumes awakened the interest of the study of porous materials, in which substantial fraction of o-Ps atoms decays into three gamma quanta. The 3γ processes were observed by four methods: triple coincidence rate, reduction of 511 keV peak in the Ge HP gamma spectrum, valley-to-peak ratio in such a spectrum, intensity of long-lived component in the lifetime spectrum. The objects of study were Vycor glass samples with the o-Ps lifetimes from 7 to 100 ns, and MCM-41 ordered silica calcinated and before calcination.

In triple coincidence measurements the counting rate of several events per second was obtained with ≈25μCi source. It means that sufficient statistics can be collected in a reasonable time. Comparison of 511 keV peak reduction with $I_{3\gamma}$ estimate from the lifetime spectra indicates that the long-lived component intensity is exaggerated. The low energy quanta from 3γ events are detected with higher efficiency and at the stop window covering 80% of the energy range the intensity of long-lived part of the spectrum is lifted up.

The sources of distortion in 3γ intensity estimation are also discussed.

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Structure of Water + Acetonitrile Solutions from Acoustic and Positron Annihilation Measurements

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We report the results of acoustic and positron annihilation measurements in aqueous solutions of acetonitrile (CH_3CN). Hydrophobicity of the solute is discussed, as well as the possibility of describing the title system in terms of hydrophobic solvation. A new method of calculating the "ideal" positronium lifetimes is proposed, basing on the mean volume of cavities (holes) in liquid structure available for positronium pseudoatom. The results are almost identical with those obtained from molar volumes using the concept of Levay et al. On the other hand, the same calculations performed using the "bubble" model of annihilation yields very different results. It seems that either acetonitrile forms with water clathrate-like hydrates of untypical architecture, or it is too weak hydrophobic agent to form clathrate-like hydrates at all. The former interpretation seems to be more probable.

Physical Aging of Carbon-Black Filled Rubber Composites as Probed by Positron Annihilation Spectroscopy

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We have used positron annihilation spectroscopy to investigate the relaxation behavior of vulcanized and un-vulcanized rubber-carbon black composites. The samples were studied at temperatures above their glassy transitions. Changes in o-Ps intensity and S-parameter are indicative of the structural relaxation process. We have found that at room temperature, both vulcanized and un-vulcanized rubber showed no changes after ageing for about two months. While within the same period, un-vulcanized samples heated at 60^{o}C and allowed to age at room temperature showed a decrease in o-Ps intensity and S-parameter. The o-Ps lifetime also decreased after this heat treatment for the un-vulcanized samples while the vulcanized ones remained unchanged. The changes seen were reversible, however, when we stopped heating the samples. We propose that heat disordered the system and on cooling, rubber molecules formed more ordered regions, which we interpret as crystallization. Vulcanized samples remained unchanged. We also found that free volume decreases during physical deformation of pure rubber, but rubber with carbon black showed a significant rise in free volume. The lifetimes, however, remained unchanged.

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Are 3-Gamma Positron Annihilations the Basis of a New Modality in PET?

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Positron Emission Tomography (PET) is a powerful tool both in biological research and clinical diagnostics, particularly in oncology. At present, it is based on the dominating 2γ annihilation: from the registered coincident annihilation photons the time dependent spatial distribution of the radiotracer can be reconstructed. The photons are merely counted and no other properties like the lifetime or momentum distribution are recorded, which could provide information about the environment with which the positrons interact, as is the case when positron annihilation techniques are applied in other fields. One of the ways of getting hold of this information, which seems most promising, lies in the detection of 3γ annihilation photons. Although they are relatively rare compared to two-photon annihilations, they give the possibility to combine the location the radiotracer (imaging) with the measurement of the 3γ yield throughout the body. The rate of 3γ decays is proportional not only to the local concentration of the radionuclide, but also to the rates of positronium formation and quenching of ortho-positronium, which in turn depend sensitively on local chemical environment, notably the presence of oxygen. In connection with the most frequent application of PET for cancer diagnosis it may provide very useful information about the level of oxygenation in tumours.

In order to explore the full potential of the new imaging concept precise measurements of 3γ yield in biological samples with controlled oxygen content are required. The standard methods relying on sandwich samples in which the investigated material is swapped with the reference material (usually Al) with known 3γ yield are rather impractical to use with liquid or semi-liquid samples in a sealed environment and the short-lived pure positron emitters used in PET. Therefore a new method has to be established. Currently an experiment is designed which should provide indication on the variability of the 3γ annihilation probability in living organisms, especially in well oxygenated and hypoxic tissues.

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Positronium Trapping in Porous Solids: Means and Limitations for Structural Studies

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Positron annihilation techniques (PAT) became routine-like methods for structural investigation of solids but interpretation of results gained by positron lifetime spectroscopy (LT) in grainy and porous media was ambiguous. Generally, at least one long lifetime component attributed to o-Ps was observed. LT measurements with increased precision have shown the coexistence of a higher number of annihilation channels contributing to the measured lifetime distribution with several medium and long lifetime components.

The analysis of our LT data on various zeolites and crystalline micrograin powders have shown that a unique picture can be obtained assuming that the dominant process is the Ps trapping in competing “extended free volume” sites, whereas inhomogeneous regions and grain boundaries may also act as Ps-trap. As the formation of Ps may occur with overwhelming dominance, the Ps trapping will dominate the LT pattern observed.

It will be shown that the interpretation of results must be based on extensive corrections for the $3\gamma/2\gamma$ counting efficiency ratio changes. It will be discussed what limitations are posed by the Ps-trapping to the applicability of PAT to structural investigation in porous systems.

Delayed Formation and Localization of Positronium in Polymers

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Recently, a delayed positronium formation in polymers has been observed [1-2] in the age momentum correlation (AMOC) experiments. In ref. [1] the effect was explained by the sub-nanosecond processes of positronium yield in the positron blob. The authors of ref. [2] assigned it with the Ps creation from a loosely bound electron and a free positron, delayed by a time (about a few hundreds pico-seconds) needed for the positron and electron meeting. The results of present work, based on low temperature lifetime experiments for LDPE and HDPE and the ETLA model [3], seem to confirm the suggestion of Ref. [2] that the process of Ps production from the shallowly trapped electrons is the decisive reason of the observed delay. The delay, according to ETLA, is caused by a slow increasing of e^+/e^- contact density inside a precursor of positronium. Because the contact density in the quasi-Ps at its initial stage is low the annihilations occur mainly by the pick-off. When the contact density increases the intrinsic annihilations play a more and more important role. Therefore the energy dispersion of quanta, originated from the quasi-Ps annihilations, changes gradually from a high value, characteristic for the pick-off decay, to a low value, relating to the intrinsic Ps annihilations. The process should be reflected in the S(t)-curve obtained from an AMOC experiment. In Fig. 1 the S(t) shapes predicted on the basis of ETLA analysis of HDPE spectra measured at 70 K are shown. The calculated shapes are very similar to the AMOC experimental data [2]. for HDPE after its long irradiation at 30 K and after bleaching the sample by light. This agreement seems to be a strong argument for validity of the ETLA analysis.

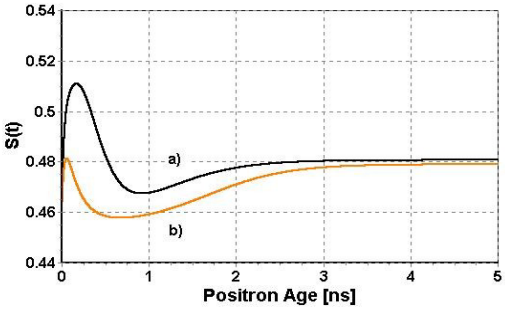

Fig. 1. The calculated shapes of S(t) curves for HDPE at 70 K a) after 70 h irradiation of sample and b) after bleaching the sample by light. In the calculations the ETLA parameters, determined from experimental spectra and some assumed values of S, i.e. 0.676 for intrinsic annihilation of Ps formed in spur, 0.95 for intrinsic annihilation of Ps formed from a positron and a trapped electron, 0.453 for free positron and pick-off annihilations, were used.

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Different Ways of Dealing with Compton Scattering and Positron Annihilation Spectra

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We present different ways of dealing with one-dimensional (1D) spectra, measured e.g. in the Compton scattering or angular correlation of positron annihilation radiation experiments. On the example of divalent hexagonal close packed metals we demonstrate what kind of information on the electronic structure one can get from 1D profiles, interpreted in terms of either 2D or 3D densities.

2D and 3D electron (or electron-positron) momentum densities are reconstructed from merely two and nine Compton profiles, respectively. Applied reconstruction techniques are equivalent, being particular solutions of the general (i.e. in *N*-dimensional space) Radon transform in terms of orthogonal Gegenabauer polynomials [1,2]. The analysis is performed both in the extended **p** and reduced **k** zone schemes.

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Many-Body Effects Observed in the Positron Annihilation Experiment

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The paper is devoted to study many-body effects, both electron-electron (e-e) and electron-positron (e-p) correlations, in the positron annihilation experiment. Our studies [1-3] showed that the static part of the direct e-p interaction (so-called enhancement) is in the best agreement with the Bloch Modified Ladder (BML) theory [4] and the e-e correlations are observed not only in the Compton scattering but also in the positron annihilation experiment. Such observations are important for the following reasons:

1^0 - all e-p annihilation theories (e.g. [5] and references therein), apart from the Arponen-Pajanne theory [6], are based on the assumption that the dynamic parts of the direct e-p and e-e interactions cancel themselves and in the positron annihilation experiment one should observe only the static part of the e-p interaction,

2^0 - all theories, except BML [4], ignore the influence the lattice potential (so called intraband and interband transitions) on the e-p interaction .

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Modified Positron Annihilation Model for Glassy-Like As_2Se_3

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A principally new approach to structural characterization of chalcogenide semiconducting glasses, based on nanoscale void-species distribution within glass-forming network, is developed for the first time.

The results of positron annihilation lifetime measurements for glassy-like g-As_2Se_3 (in our experiments with ORTEC spectrometer, the full width at half maximum was 0.270 ns and ^{22}Na isotope was used as a positron source) are compared with free-volume nanovoid distribution for 146-atoms layer-biased computer model, obtained with Monte Carlo simulation method. It is shown that defect-related positron lifetime of 0.37 ns within two-state positron trapping model (the obtained spectra were fitted by LT program of J. Kansy) corresponds to the group of free-volume nanovoids with average radius of 2.9 Å.

The same value can be obtained from X-ray diffraction patterns of g-As_2Se_3 taken in respect to the first sharp diffraction peak (FSDP), which is a characteristic feature in the measured structure factor of many disordered solids. Ascribing FSDP to a chemical-order pre-peak in the concentration-concentration partial structure factor, arising from the clustering of interstitial nanovoids around cation-centered units (Elliott's model), it was shown that, in the case of *g*-As_2Se_3, the FSDP position and nanovoid diameter were connected through a coefficient close to 2π that is a typical situation for X-ray reflexes from crystallographically-ordered atomic planes. It probably means that the FSDP-related free-volume nanovoids form interlayer separation regions in a glass network.

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Defects in Semiconductors Studied by Positron Annihilation Spectroscopy

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Positron research of semiconductor defects is now intensively done for more than two decades. The peculiarities of positron trapping in semiconductors appearing due to the Coulombic interaction of the positron with charged defects are in the meantime relatively well understood. Thus, PAS became a very useful standard tool for defect characterization in semiconductors [1].

In the talk, prominent examples of semiconductor defect studies of the Halle positron group of the last 20 years will be presented. This will include elementary semiconductors as well as II-VI and III-V compound semiconductors in the as-grown state and after intentional damaging (low-temperature electron irradiation, plastic deformation) using all techniques of positron annihilation.

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EPOS – an Intense Positron Beam Project at the Research Center Rossendorf

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EPOS means ELBE Positron Source. This project will become an intense positron beam of monoenergetic positrons (0.2 … 40 keV) for materials research applications. The beam will be bunched for positron lifetime spectroscopy. It makes use of the primary bunch structure of the ELBE electron beam (77 ns repetition time, cw mode, 40 kW, 40 MeV). The system will be built as external, user-dedicated facility of the University Halle at the ELBE Radiation Source of the Research Center Rossendorf. In the talk, the concept of the system will be introduced and they main components will be discussed (positron converter and beam dump, beam guidance system, bunching system and multi-detector arrangement). The results of different Monte-Carlo simulations of the beam will be shown (electron-positron conversion, beam trajectories, and bunching system). The expected beam parameters will be presented.

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A Free Volume from Positron Annihilation Lifetime Spectroscopy and Dynamics of Glass-Forming Systems

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The o-Ps annihilation responses of organic small molecular and simple polymer systems will be presented. An example of correlation between effective free volume hole characteristics and macroscopic dynamics will be demonstrated on the cases of dielectric relaxation data of glycerol and poly(propylene glycol).

An attempt to describe the temperature dependence of free – volume from PALS in super-cooled liquid will be presented.

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Free Volume in Polymeric Membranes: Comparison of Positron Annihilation Lifetime Spectroscopy and Evaluation of MD Simulations

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Gas separation by membranes is important for many technical applications. The amount and distribution of free volume in polymeric membranes significantly determines the transport and separation properties. In the present work these free volume characteristics were determined directly from MD simulations via a new method [1,2]. Here a "tracer atom" probes the simulation cell to determine the non-occupied volume. On the other hand the positron annihilation lifetime spectroscopy was used to determine the average size of free volume cavities via a well established correlation between ortho-positronium lifetime and size of the cavities. Characteristic results for polyimides will be presented, comparison of both methods will be made, and limitations of the standard model for the evolution of the positron lifetime data will be discussed.

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Positron Annihilation Lifetime *in situ* Study of Deformed Polyolefin Elastomers.

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Engage (commercial name) polyolefin elastomers are ethylene octene copolymers which exhibit excellent physical properties including elasticity, toughness, and low temperature ductility.

The positron annihilation lifetime measurement has been employed for four samples of this copolymer of different octene monomer content. The samples were deformed at room temperature in the range from 0 to 110 % and for each degree of deformation a series of PALS spectra was collected *in situ.* The total statistics of the spectra making up a series was not less than 10^7 counts. To increase the unambiguous of obtained results of numerical analysis all the spectra in such a series were fitted simultaneously by LT [1] program with the same theoretical model of identical PALS parameters.

The radius (R) of free volume holes as a function of deformation has been studied (Fig. 1).

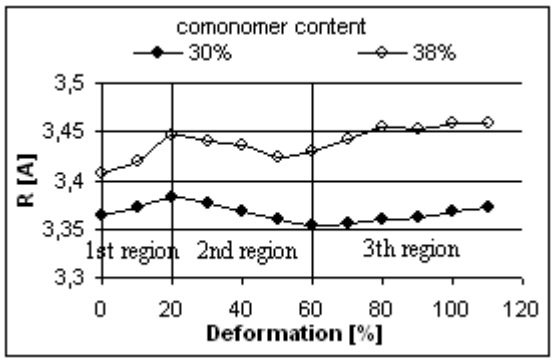

Fig. 1. The variations of free volume hole radius as a function of deformation in ethylene octene copolymer of different comonomer content.

The variation of R with deformation shows three stages [2], which, on the basis of comparison with the stress strain curve, can be assigned to elastic stage, strain-softening and plastic region. In the light of these variations the changes of microscopic polymer structure are discussed.

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Calculation of Positron Response from Embedded Nanoparticles

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Embedded nanoparticles can be effectively studied by means of positron annihilation because they can trap positrons under favorite conditions. Positron annihilation characteristics then contain information related to nanoparticles' electronic and atomic structure. Of great importance is to calculate the positron response from such nanoparticles that can be compared with experimental data. In this way nanoparticles can, in principle, be identified.

As such calculations based on the first principles methods are computationally very demanding, a method based on the atomic superposition technique was developed recently [1], which allows to determine positron characteristics with much less computational effort compared to first principles techniques. This method is explained in detail, justified on the basis of first principles calculations, and applied to Cu nanoparticles in Fe. The advantages of the above mentioned method are demonstrated for the case of a precipitation study of Cu in Fe. Examples of other systems are given as well.

This work has been funded within the 6th Framework Program under the Integrated Project PERFECT (FI6O-CT-2003-508840).

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Carbon Thin Films Deposited on Si and PET: Study of Interface States

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Diamond like Carbon (DLC) films are intensively studied because of their many useful properties like chemical stability, biocompatibility, optical transparency in the visible, high thermal conductivity, high electrical resistivity and gas barrier capability. Their use is limited to few industrial niches (magnetic recording, wear protection and antireflective coating) but now they are entering the field of biomedical, electronic application and packaging.

We have performed, by Positron Annihilation Spectroscopy, a characterization of thin carbon film deposited at the same condition on different substrates (Si and PET) with the aim to compare their open volume structure and possible different interfacial states. The open volume structure of these films is important because affects their mechanical properties (hardness and stress). The interfacial states are fundamental for the adhesion of the films and for their use in electronic devices.

Carbon films were deposited on (100) Si wafers and PET. The deposition was carried out at room temperature in a capacitively coupled RF-PECVD system (13.56 MHz) using a mixture of CH_4-CO_2 as gas precursor. The cathode was the RF powered electrode (V_{RF} = -300 V), while the substrate for growing the film was mounted on the anode without application of any external bias (V_{BIAS}). The deposition was operated at pressure of 0.2 Torr.

PAS was carried out with a slow positron beam coupled to a Doppler Broadening spectrometer to measure the S parameter as a function of the positron implantation energy. The data have been analyzed by the VEPFIT program.

The films, both grown on Si and on PET, are homogeneous as regarding the open volume distribution. Conversely, the carbon films have been found to modify the electric field at the carbon/Si interface.

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Commercial Application of Positron Annihilation

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Industry is increasingly becoming attracted to the unique annihilation properties of positrons and positronium. Since they are charged particles and can be precisely controlled by electric and magnetic fields, their unique interactions with ordinary matter and their lack of residual radiation after annihilation lend them to many practical and potentially lucrative commercial applications. This talk will discuss some of those applications in the areas of space propulsion, medical and material science uses. The advantages and disadvantages of using positrons and positronium as contrasted with other techniques in these fields will also be discussed.

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A Molecular Model for Geometry Relaxation and Annihilation Rates of Positron Complexes

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A molecular model for positron (e^+) complexes with atoms and molecules, in which e^+ is treated as a light nucleus is presented. We consider that the electronic and nuclear (including e^+) motions are separable and assume an adiabatic (product type) wavefunction for a complex. In the variational adiabatic approximation with a model Hamiltonian the isotope (finite nuclear mass) effect is taken in account in the attainment of the electronic wavefunction and the potential energy surface (PES) for nuclear motion. The model is explored to obtain the e^+ bonding site and relaxed molecular geometry due to e^+ attachment, at the minimum of the PES [1,2]. Examples will be presented for [LiH; e^+], [urea; e^+] and other complexes. The PES permits to study the complex "dissociation" as well, for large molecule-e^+ distances and informs whether the process yields a bare e^+ or a positronium as a dissociation product. This information is used to analyze the data on annihilation rates in the literature [1]. We are considering applications to rationalize data from e^+ spectroscopy or scattering experiments as well.

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Non-Destructive Lifetime Prediction Using the BPM

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For the construction of mechanical components it is essential to know the lifetime of the sample under dynamical load conditions.

Positron Annihilation Spectroscopy measurements in iron steel (X6 CrNiTi 18-10, C45E) and titan Ti2 show a linear dependency on the S-Parameter and a logarithm of the cycle number [1]. Iron based materials fail at a critical defect density independent of cycle number and load. The defects can be used as precursors to extrapolate the remaining lifetime of the sample.

Using special sample geometries with different stress states along the sample axis and employing the fine focus positron beam of the BPM [2] we can predict the lifetime for different loads on a sample.

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Embedded Nano-Clusters: Coincidence Doppler Broadening and 2D-ACAR

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The advantage to use *positron* to analyze nano-clusters embedded in materials originates from its "self-seeking" and "site-selective" behavior. If there is any positron affinitive site in the material (typically more than few ppm in number density), thermalized positron is sensitively trapped at the site during the diffusion, and then annihilates with one of the electrons around the trapping site. By detecting annihilation gamma photons, we can obtain exclusively information on the trapping site sensitively.

It is well known that vacancy-type defects are such positron affinitive sites because positively charged nuclei are absent there. However, they are not the only positron affinitive site. Recently, we have found, using coincidence Doppler broadening (CDB) spectroscopy, that some kind of nano-clusters embedded in materials without any open volume defect can also trap positrons sensitively, which expands the applicability of positron annihilation in material science.

In this lecture, our recent results on embedded nano-clusters by using the CDB and 2D-ACAR method will be presented: 1) Vacancy-Cu aggregations and defect-free bcc Cu nano-clusters in Fe formed by irradiation and thermal aging [1-3], 2) fcc Zn and Ag clusters in Al alloys [4]. Some of them are compared with the results by other techniques such as transmission electron microscopy and three-dimensional atom probe field ion microscopy, and the smearing of the momentum distribution in the nano-clusters due to the nano-size effect is discussed.

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A Real Time S-parameter Imaging System

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Obtaining lateral S-parameter image scans for positrons implanted into semiconductor devices or biological specimens can be a helpful research tool both in discerning function and in diagnosing defect patterns that could help interpret function. S-parameter images can be obtained by either mechanically scanning small positron emitting isotopes or by electromagnetically rastering a controlled energy positron beam of small spot size across the sample. In the former case and image of the top 10-100 micron (depending on density) of the sample sub-surface can be obtained. In the latter case images at different depths (ranging from 1nm to 10 micron) maybe obtained. Here we describe a general hardware and software architecture of relatively low cost that has recently been developed in our laboratory which allows the whole sub-surface S-parameter image to be obtained in real-time. This system has the advantage over more conventional sequential scanning techniques of allowing the operator to terminate data collection once the quality of the image is deemed sufficient. Examples of various S-parameter images taken on various devices at different depths are shown which demonstrate the potential and usefulness of this type of imaging architecture.

Defect Characterization of BF_2 Implanted Silicon Samples by Positron Annihilation Spectroscopy

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Researches on smaller device dimensions in electronics require precise analysis of defects. BF_2 molecular ion implantation into silicon has the advantages of higher electrical activation and lower leakage current for P/N junctions. In this work, BF_2 implanted silicone samples produced at different implantation energies, 3 keV, 5 keV and 10 keV, are analyzed by Slow positron beam (0-40 keV and 10^5 e^+/s) (Variable Energy Positron (VEP)) at the Positron Centre Delf. The measured line shape parameters, S and W, corresponding to annihilation of positrons, give valuable information about the defect profile of the sample material enabling the optimization of the manufacturing process according to the annealing temperature and the ion implantation energy.

Positron Annihilation in Defected Monocrystalline Gold Samples

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Angular distributions of the positron annihilation quanta were meassurement for monocrystalline gold samples, oriented in (100), (110) and (111) directions. The samples were deformed by elongation for different deformation degrees. The S and W parameters as a function of deformation degree of the sample have been determined. It was found that the dynamics of the dislocations and vacancy generation during the sliding of some crystallegraphic planes, depends on the crystallgraphic direction.

Construction of a Relativistic Positron Beam at a Van de Graaff Accelerator for *in situ* Lifetime and AMOC Measurements

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At the University of Gent a relativistic positron beam at a 2.5 MeV Van de Graaff accelerator is under construction. This beam is constructed to perform high count rate positron lifetime measurements and AMOC experiments. It will be used to study metallic and polymer samples under deformation.

We propose to use a Canberra PIPS detector as a ΔE start detector and we will discuss the advantage of using this detector with a thickness 500 μm in comparison to a thin plastic scintillation detector [1].

A new electrostatic positron injector was designed based on a transmission single crystal Wolfram moderator. The combined performance of the injector and complete transport system was simulated using the SIMION 6.0 program [2]. The results of the beam characteristics are presented.

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Positron Annihilation in Medical Preparations of Insulin

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Positrons lifetimes were measured in medical preparations of insulin (human and animal), differing as far as the degree of purity and time of their activity in the organism are concerned. In all of the cases the spectrum of positrons lifetimes was distributed into three components, with the long-life component ranging from 1.8 to 2.08 ns and the intensity taking on values from 18 to 24%.

Making use of Tao-Eldrup model, the average radius of the free volume, in which o-Ps annihilated, and the degree of filling in the volume were determined. It was found hat the value of the long-life component for human insulin is higher than that of animal insulin. Moreover, the value of this component clearly depends on the manner of purification of the insulin. It was also noticed that there occurs a correlation between the value of this component and the time after which it begins to be active in the organism, as well as the total time of its activity.

Low-Energy Cross Sections for Positron Interaction with Cyclic Hydrocarbons

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Total cross sections for positron scattering on benzene, cyclohexane and aniline have been measured by a slow beam at 0.4-20 eV collision energy. The cross sections rise in the limit of zero energy, reaching surprisingly high values, say $1x10^{-14}$ cm^2 at 1.5 eV in benzene and aniline. Theory of Occhigrossi and Gianturco [1] predicts well this trend, but underestimates the values by a factor of two. In cyclohexane the cross section is lower by 20% than in benzene; in the limit of zero energy it tends to a constant value. In aniline and benzene some shoulder structures are observed near to thresholds for positron annihilation, indicating cross sections for positron formation of about $5x10^{-16}$ cm^2.

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Replica of ortho-Positronium Characteristics when Using the Programme LIFETIME

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When using the positron lifetime spectroscopy in polymer research a question arises of good reproduction of a free volume distribution. The latter may be obtained from a positron lifetime distribution (PLD).

In the past such computer codes as CONTIN and MELT have been used in the continuous lifetime analysis. However lately the programme LIFETIME is often used to this aim. The opinion has been given that one can avoid the shortcomings of CONTIN and MELT using LIFETIME [1]. In the programme the log-normal distribution of the annihilation rates is assumed.

One is particularly interested in reliable information on the FWHM of very narrow and broad PLDs. Great difference in the width of distributions are often found when research covers a wide range of temperature.

In the paper results of the analysis of lifetime spectra performed by students with use of the programme LIFETIME v.9 are presented [2]. Three-component lifetime spectra with the log-normal o-Ps lifetime distribution have been simulated. The input values of lifetimes τ_1=0.125 ns , τ_2= 0.4 ns, τ_3=1.5 ns and intensities I_1= 10% , I_2= 70% , I_3= 20% are close to values of frequent occurrence in polymers, e. g. in polyamide 6, studied by us [3]. The input value of the FWHM of the lifetime resolution function, assumed to be a gaussian, was equal to 0.270 ns. The input values of the standard deviation of the o-Ps lifetime distribution changed from 0.05 ns to 0.8 ns, while the total number of counts was between $1 \cdot 10^6$ and $30 \cdot 10^6$. No constraints were imposed. All parameters were free. Good replicas of the ortho-positronium characteristics have been obtained for standard deviations greater than 0.3 ns and the total number of counts greater than$1 \cdot 10^6$.

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Electron-Positron Momentum Densities for Electrons from Individual Core Levels

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Recent experiments demonstrate that application of positron annihilation induced Auger electron spectroscopy combined with Doppler broadening technique makes it possible to map with quite a good accuracy the electron-positron (*e-p*) momentum densities for electrons from individual core shells [1]. In the present contribution I focus on various effects affecting the slope of calculated spectra for core electrons. In particular, influence of positron distribution, of approximation used for the *e-p* correlation functions, as well as of finite apparatus resolution on the core part of the *e-p* momentum density is discussed.

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Positron Annihilation in Polycrystalline Metals Deformed by Uniaxial Tension

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Angular distributions of the positron annihilation quanta were measurement for polycrystalline samples deformed by uniaxial tension up to different deformation degrees. The S parameter as a function of the W parameter has been determined. The data obtained for samples elongated up to different elongation degrees indicate that in the proportionality and limited proportionality regions the changes in the physical properties of samples are governed mainly by generation of vacancies and formation and kinetics of transformations of vacancy clusters occurring first of all on the grains of monocrystallites. In the region of plastic deformations the dominant defects are dislocations and vacancies and their aggregates generated due to the formation and movement of the dislocation of the primary and secondary slip. The positron annihilation dates are corroborated by the results of the resistometric and tensometric measurements in the proportionality and limited proportionality region.

Influence of Experimental Noise on Densities Reconstructed from Line Projections

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The influence of experimental noise on densities $\rho(\mathbf{p})$ reconstructed from their plane projections (Compton profiles) was investigated in papers [1]. In this contribution the same problem is studied for line projections of $\rho(\mathbf{p})$ (2D ACAR spectra). We performed simulations of statistical noise for many sets of 2D spectra of two different model $\rho(\mathbf{p})$ with the cubic symmetry. The densities were reconstructed using the Cormack method [2] and, finally, the error propagation in terms of standard deviations, $\sigma[\rho(\mathbf{p})]$, was estimated. We observe that the distribution of $\sigma[\rho(\mathbf{p})]$ has its extremes along the main symmetry directions and also a tendency to accumulate for small p, in agreement with the results in Ref. [1]. Moreover, we noticed that the more density components, $\rho_n(p)$, have to be taken to description of $\rho(\mathbf{p})$ the less anisotropic is the distribution of $\sigma[\rho(\mathbf{p})]$.

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Some Aspects of Free Volume Studies in Molecular Substances Using Positron Annihilation Experiments

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It is accepted now to use positron annihilation lifetime (PAL) method for the studies of elementary free volume holes in solids (in polymers in particular). The aim of this report is to discuss some problems met on this way and to illustrate them by the results of the authors.

(1) Some small admixture of polar groups, especially included in conjugated systems, may cause strong inhibition of Ps formation at various temperatures. Thermostimulated luminescence (TSL) experiments and coincidence of the Doppler broadening spectra (CDBS) show that the effect is explained by the trapping of electrons as well as positrons and is not associated with the number of the free volume elements. Clearly pronounced limit of inhibition in the case of ethylene-methylmetacrylate copolymer infers that some fraction of epithermal positrons may take part in positronium formation in the spur. **(2)** Mentioned above effect and also examples when intensity of the long-lived ortho-positronium component I_3 is determined by the density of electrons in the positron spur rather than by the amount of free volume holes make this intensity unacceptable parameter for the free volume studies. Measurements of temperature dependences of annihilation characteristics and of the specific volume are much more effective for calculations of the number density of the free volume holes *N(R)*. This approach is illustrated on example of polyimides. **(3)** Super-cross-linked polymer sorbents (made on the bases of polystyrene) with extremely low density (about 0.5 g/cm^3) and very developed specific surface (1400 m^2/g) are of special interest; o-Ps lifetime distribution consists in this case of several components, the longest surpassing 70 ns. Free volume holes in the polymer sorbents were so large that a comparison of *N(R)* obtained from the PAL investigations in combination with apparent density measurements and that from the low-temperature nitrogen sorption experiments (treated using Brunauer-Emmett-Teller theory) accomplished by the NITTO DENKO Corporation became possible. Such a comparison seems to be useful for checking of contemporary theoretical models explaining temperature dependence of annihilation characteristics in the holes of extra-large size.

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PAL Spectroscopy as Void-Species Structural Probe for Multifunctional Spinel-Type Ceramics

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The main aim of this work is to develop a meaningful interpretation of positron annihilation lifetime (PAL) characteristics for multifunctional ceramics at the example of mixed transition-metal manganite ceramics of $Cu_{0.4}Ni_{0.4}Co_{0.4}Mn_{1.8}O_4$ chemical composition and alumomagnesium $MgAl_2O_4$ ceramics with a spinel structure obtained with a traditional ceramic technology route.

In our PAL-experiments with ORTEC spectrometer, the full width at half maximum was 0.270 ns and ^{22}Na isotope (0.74 MBq) was used as a positron source. The obtained spectra were fitted by LT program of J. Kansy. Especial procedure was applied for the first time to develop a phenomenological model for multi-channel positron annihilation channels in the investigated ceramics.

It is concluded that only three-component fitting procedure is the most suitable one for all cases under consideration, these extended free-volume defects being as follows:

- positron traps in the form of individual vacancies and small vacancy-like clusters, attributed to the shortest PAL component;
- positron traps in the form of extended vacancy-like clusters, powder particle surfaces, large-angle grain-boundaries, attributed to the middle PAL component with $\tau_2 \approx 0.25$-0.50 ns;
- nanostructured free-volume voids in ceramics bulk (presumably, between individual grains owing to incomplete intergranual contacts), which can capture positronium atoms.

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Complex Intermetallic Compounds: Defects, Disordering, Details

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A short overview will be given on the thermodynamics of the formation of thermal defects in intermetallic aluminides. We focus on thermal vacancies [1] studied by the specific techniques of positron annihilation [2] and time-differential dilatometry [3] and discuss the results together with self-diffusion data [4]. We then demonstrate that these techniques can be employed for studying vacancies in compound semiconductors specifically [5]. Furthermore, structural order-disorder phase transitions can be investigated from an atomistic point of view [6] by making use of positron annihilation as shown in the exemplary case of Al-Ni-Co quasicrystals. A few examples for the application of intermetallics will be given in the introductory part.

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Electron-Positron Interaction in Metals. Theory and Experiment

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The electron-positron interaction greatly complicates the interpretation of positron annihilation data. The two-detectors Doppler measurements of Mijnarends et. al. as well as our theoretical calculations point at the conclusion that the local density approximation to e^+-e^- interaction is a good way of treating this problem in real metals. This shows that e^+-e^- interaction in an electron gas is the key to understanding this phenomenon also in inhomogeneous systems. On the basis of dozens of experiments one comes to the conclusion that the well known formula of Boroński and Nieminen for the electron accumulation on the positron in jellium describes the best the positron lifetimes in metals. However, it is based on the calculations of Lantto which start from physically controversial assumptions. Moreover the results of Lantto obtained using the Fermi hypernetted-chain (FHNC) approximation are not confirmed by more recent Monte-Carlo calculations. The results of Arponen and Pajanne, of Rubaszek and Stachowiak and of Stachowiak and Lach lead to too short positron lifetimes. The discrepancy is of the order of 8 to 15% for r_s =2. This shows that we still do not fully understand e^+-e^- interaction even in an electron gas.

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Role of Trapped and Solvated Electrons in Ps Formation

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Role of trapped and solvated electrons in Ps formation is discussed. Combination of thermalized positron with such electrons is energetically possible and may contribute to Ps formation. Contrary to the positron reaction with a quasi-free electron, this process is not limited to picosecond times, but proceeds on a timescale of nanoseconds. In this case conventional exponential deconvolution of row lifetime positron annihilation spectra becomes questionable. Rigorous treatment of the data needs nonexponential deconvolution, based on an adequate physical input. Such an approach is suggested here. Its reduced form is used for interpretation of the Ps formation data in polyethylene, EMMA and PMMA in dark and in light vs. time of the measurement and temperature. Parameters characterized accumulation of trapped electrons and their recombination with counter ions and positrons are obtained.

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Revision of the Model of Radioactive Hydrogen, Hydrated Electron and Ps Formation in Aqueous Solutions. First example of the Ps enhancement effect

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Behavior of the yields of the solvated electrons, G_e, radiolytic hydrogen, G_{H2} and G_H, and positronium atom, P_{Ps} vs. concentration c_S of the solute S (electron scavenger) in aqueous solutions is reanalyzed in the frameworks of the diffusion-recombination model (blob model). The developed theory explains from a common viewpoint

1) experimental data on accumulation kinetics of intermediate (e^-_{aq}, H, OH, Ps) and final (H_2, H_3O^+, OH^-) in pure water, and concentration variation of the yields in solution of various (first of all electron) scavengers;

2) experimentally established quasi-exponential decrease of the e^--yield:

$G_e \approx G_e^0 \exp(-c_S / c_{37})$;

3) the so-called "cube-root-low" for H_2: $G_{H2}^0 - G_{H2}(c_S) \propto c_S^{1/3}$ at small c_S and proportionality of $G_{H2}^0 / G_{H2}(c_S)$ to c_S at larger concentrations;

4) insensitivity of the H_2-yield in acid solutions.

Yields of H_2, Ps and luminescence in water-acetone and alcohol-acetone solutions are experimentally measured. Interpretation of these data together with G_e, G_{H2} and P_{Ps} in aqueous solutions of NO_3^-, H_2O_2 and $HClO_4$ allows to prove that acetone molecules, being dissolved in water, capture track electrons and form weakly bound state Ac^-, which may then transfer its electron to the positron, and promote Ps formation. It is the first demonstration of the Ps enhancement effect in a polar solvent.

Our consideration says against a very short lifetime ($\leq 5 \cdot 10^{-14}$ c) of the primary radical-cation H_2O^+. There is some indication of contribution of e^-_{aq} to the Ps formation.

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Interactions of Antihydrogen with Hydrogen and Helium

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The planned measurement of the antihydrogen (AH) spectrum, which should make possible checking of predictions of the Standard Model with high accuracy, will require storing of substantial amounts of AH at subkelvin temperatures. The processes of interaction with normal matter - scattering, creation of bound states, annihilation, „chemical reactions" – lead usually to AH losses. There is, however, an idea that AH could be cooled in collisions with ultracold atoms and molecules.

The potential energy functions will be presented for H-AH, He(^{1}S)-AH, He(^{3}S)-AH and H_2-AH interactions. They are the first step for theoretical studies of the processes mentioned above, within the adiabatic and Born-Oppenheimer approximations. The variational approach was used in the calculations, with the basis of explicitly correlated Gaussian functions. Problems, which appear for the systems, like H-AH and He(^{3}S)-AH, will be discussed. For these systems, the leptonic ground state wave function does not describe a bound state below the so-called critical internuclear distance (R_c). The adiabatic approximation breaks down in the vicinity of R_c.

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Application of Coincidence Doppler Broadening Spectroscopy to Polymers and Hydrocarbon Samples

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Positron annihilation lifetime spectroscopy (PALS) and measurement of the Doppler-broadened annihilation line (DBAL) are used simultaneously very often resulting in better understanding of annihilation processes. Positronium (Ps) formation yield in polymers is affected by many factors like: size of intermolecular spaces, chemical structures, crystallinity, radiation, and temperature. Although the lifetime of free positrons, positrons not taking part in Ps formation, is quite constant and unaffected by these factors, the information obtained by DBAL may be more valuable because the energy spectra measured by DBAL carry information about the electron momentum distribution of the studied sample.

Using two Ge detectors, Doppler-broadened energy spectra can be obtained by measuring the coincidences of the two annihilation photons. This technique is known as coincidence Doppler broadening spectroscopy (CDBS) and used by many positron groups for metal studies. The peak to background ratio is significantly improved and reaches 10^7, and the high-momentum part of the energy spectrum, which is related with annihilation of positrons on core electrons, can be resolved out. From this information, even a small fraction of elements different from the constituent atoms of the studied sample can be detected. However, for the case of polymer study, Ps formation usually occurs what changes the CDBS spectrum and makes the extraction of the electron momentum distribution difficult. Using the common relation between the free positron fraction and the Ps yield, the electron momentum distribution can be extracted from the CDBS energy spectrum for polymers.

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Testing the ETE Model. Silica Gels Produced with Polymer Template

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In the framework of testing the extended Tao-Eldrup model (ETE) the measurements of temperature dependence of the o-Ps lifetime in porous media were performed. The samples were silica gels produced with the use of polymer templates. The composition of polymer and TEOS solution, and the temperature of aging allow to produce the silica gels with various pore diameters.

In the case of gel with R = 2.0 nm the lifetime variation with temperature follows roughly the model predictions; the model curve runs between the PALS data for lifetime at the peak of distribution and mean lifetime value. However, the tendency to larger $\partial\tau/\partial T$ is observed. The result is similar to that for Si40 (Merck) silica gel, obtained previously [1,2].

For the samples with smaller R that strong dependence on temperature is augmented, contrary to the model expectations. At pore radius 1 nm all positrons should annihilate from the ground level and the lifetime should be roughly constant. The experiment shows that at low temperature an additional, unexpected component dominates; its intensity drops to ≈10% from 250 K upwards, but the lifetime reaches 90 ns, while LN adsorption does not indicate the presence of bigger pores.

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Studies of Opals by Use of Positron Annihilation, SEM and XrD Techniques; Application of Novel Short-Lived Positron Sources

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Positron Annihilation Lifetime (PAL) and Doppler Broadening Spectroscopy (DBS) studies on opals showed exceptionally high lifetime and S-parameter values as compared to other silicate samples of similar composition but with a different structure. The positron signal was correlated with opals' phase in diagenesis process in which opals change their structure from amorphous (opal-A) to crystalline and change their composition from water saturated to dehydrated. The analysis was done also on precious opals, characterized by uniformly sized spheres and voids structure of hundreds of nanometers in diameter in order to check the limits on positronium formation as a function of the void size.

Novel short-lived positron sources produced by gamma activation methods were successfully used. Application of improved analytical methods to DBS studies allowed a distinction between positron and positronium annihilation effects.

Scanning Electron Microscopy (SEM) and the X-ray Powder Diffraction (XrD) were used as complementary techniques to identify the diagenesis stage of opals, the type of present crystals and to estimate a degree of crystallinity/amorphicity of the opal samples.

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Perspectives on the Production of Cold Antihydrogen

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CPT conservation is one of the basic axioms underlying the Standard Model. One of the ways of verifying CPT conservation is by studying antihydrogen atoms using high resolution laser spectroscopy. In 2002 the ATHENA collaboration produced the first cold antihydrogen atoms as the initial step towards the measurement mentioned above. Over the last two years progress has been made in the investigation of antihydrogen production. Here we will describe the process from positron and antiproton trapping, positron transfer and stacking to detection of the neutral antihydrogen atom. Furthermore the production mechanisms will be discussed. A brief outlook for the near and long term future will be given.

Nanostructures: Simulation and Experiment

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The reduction of the grain size down to the nm regime has opened new and fascinating avenues for research in several aspects of materials science, including mechanical properties. In recent years large efforts, both experimental and computational, have been made to understand the deformation mechanisms at the nanoscale. Computer simulations suggest both grain boundary accommodation mechanisms and intra granular slip involving dislocation emission and absorption at grain boundaries, as possible deformation mechanisms. In these simulations the structure of the grain boundaries plays a crucial role.

In the past 15 years positron annihilation lifetime spectroscopy has been used extensively to investigate the defect structure at grain boundaries in nanocrystalline materials. However, grain boundaries are often composed of very complex defects structures that in principle cannot be described by one or two single positron lifetimes components. Recently we have developed a method to calculate the positron signal in very large simulated nanostructures, which enables us to gain a better understanding of the free volume distribution in grain boundaries.

We present the results of positron lifetime calculations on simulated nanostructures constructed by two different techniques and compare them with the latest experimental results. Furthermore we discuss briefly the relationship between grain boundary free volume and specific properties of grain boundaries such as the existence of local modes in the high frequency region of the vibrational density of states.

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Annealing Study of Al/GaSb Contact with the Use of Doppler Broadening Technique

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With the use of a monoenergetic positron beam, annealing study of the Al/n-GaSb contact was performed by monitoring the Doppler broadening of the annihilation radiation as a function of the positron implanting energy. The S parameter depth profiles were successfully fitted by a three layer model (Al/interface/GaSb). The annealing out of the open volume defects in the polycrystalline Al overlayer was revealed by the decrease of S_{Al} and increase of $L_{+,Al}$. The increase of $L_{+,interface}$ (and the decrease of $S_{interface}$) upon annealing suggests the reduction of open volume defects (for example dislocations and vacancies) in the intefacial region. It is observed $L_{+,GaSb}$ firstly increases and then decreases with increasing annealing temperature. The increase of $L_{+,GaSb}$ is due to the annealing out of the V_{Ga}-related defect. The subsequent decrease of $L_{+,GaSb}$ upon further annealing is possibly due to the formation of a new vacancy-Te defect complex, for which the data of XPS measurements also agrees with such speculation.

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Positron Annihilation Lifetime and Coincidence Doppler Broadening Study of γ-Irradiated Polyethylene

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We performed simultaneous positron annihilation lifetime (PAL) and coincidence Doppler broadening (CDB) measurements on γ-irradiated high-density polyethylene (HDPE) at different temperatures. It is shown that at room temperature, more than one order of magnitude larger free radical concentration (from ~10^{17} to 10^{18} spins/g) result in a reduction of the *ortho*-positronium (*o*-Ps) yield by only ~2% for HDPE irradiated in vacuum. Stronger inhibition of Ps formation was observed in HDPE irradiated in air, which is attributed to the trapping of both electrons and positrons by oxygenated species. In contrast to the room temperature measurements, correlation between irradiation-induced chemically active species and PAL results turn difficult at 373 and 80 K. It was revealed that in the former case, a rapid decay of free radicals didn't lead to any clear change in the *o*-Ps yield within the extended measurement time as long as 100 h; and in the latter case the obtained CDB spectra for specimens irradiated under different conditions are quite similar. Detailed discussions will be given at the conference.

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Positronium Formation in Solid Long-Chain Alkanes

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This paper represents a fragment of systematic studies on positron annihilation in solid saturated hydrocarbons (alkanes, paraffins) from $C_{17}H_{36}$ to $C_{31}H_{64}$. The Tao-Eldrup model and its extensions allow identifying the regions in crystalline structure where positronium is trapped, and estimate respective trap sizes. A variety of phases is observed in these hydrocarbons. In the rigid phase I positronium locates mainly in two-dimensional empty space between the lamellae of crystal structure. Additional free volumes exist in high temperature phases due to appearance of intramolecular defects. There are a few *n*-alkane conformers: *all-trans, end-gauche, double-gauche* and *kink*. Each of them, except *all-trans*, represents a nonplanar molecule distortion. In consequence free volumes of different sizes appear.

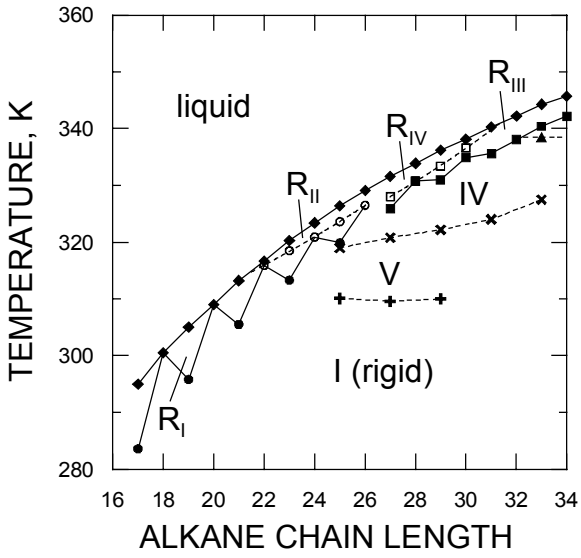

Fig.1 Phase diagram for n-alkanes.

The rise of o-Ps intensity with the sample irradiation dose, which was seen earlier in polymers [1], is observed also in *n*-alkanes. One can find similarities between the o-Ps annihilation in crystalline alkanes and polymers, like exponential character of that rise, and the trap bleaching by illumination. It confirms the same origin of the intensity growth, i.e. the accumulation of trapped electrons. Two kinds of electron traps were found. The time constant of electron accumulation in the traps depends on the carbon chain length and varies with temperature in different way for even and odd-numbered alkanes.

Odd-even differences at supercooling are also mentioned.

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Surface Deformation on a GaAs Wafer Resulting in Point Defects – Is the Identification of the Sublattice Possible?

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Scratches on the surface of an undoped semi-insulating GaAs wafer have been produced by a wedge-shaped single diamond grain. The subsurface damage has been analyzed by the Bonn positron microprobe [1]. This instrument provides laterally resolved positron annihilation measurements, which are sensitive to lattice defects like vacancies and dislocations. Analyzing the high-momentum part of the annihilation radiation, we try to identify the sublattice of the detected defects by a comparison to calculated positron annihilation parameters as in [2,3]. We can clearly identify different regions of damage, which have been characterized both by conventional scanning electron microscopy and the positron microbeam. The latter reveals indications of plastic deformation due to the trace of created defects observed [4]. We discuss the possible implications of the observed ductile behavior of GaAs usually known to be brittle at room temperature and under atmospheric pressure.

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Positronium in Solid n-Pentacosane

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Positron annihilation lifetime spectra in solid *n*-pentacosane (saturated paraffin $C_{25}H_{52}$) were measured as a function of temperature and positron irradiation time. It was found that phase IV, occupying at heating the range of 0.7 K only, becomes well visible in the cooling runs due to easy supercooling of that phase; small increase of ortho-Ps lifetime in phase IV comparing to low-temperature one indicates that dominant intramolecular defects are *end-gauche* ones. In both rotator phases the lifetime value results from high concentration of *kink*-type conformers. Transition from phase I to V is not visible in the lifetime spectra.

The effect of accumulation of excess electrons leading to the rise of o-Ps intensity with time, typical mainly for polymers, was also observed. Two kinds of electron traps were found. Main trap component has the activation enthalpy 0.6 eV and detrapping process is completed at about 250 K, the time constant of I_3 rise is about 6 h. Additional fast accumulating component (time constant of about 1 h) exists up to the temperatures near the transition to the rotator phase.

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Defects in Silicon Studied by First Principle Method

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Positron-Electron momentum density functions for different defect sites of silicon such as V,VX,VX2 have been obtained from first principle all-electron calculations where X is the dopant P,As or Sb. Calculations were based on the two component density functional theory under both the local density approximation(LDA) and generalized gradient approximation(GGA). The electron wave functions were calculated using the full potential linearized-augmented-plane-wave (FLAPW) method. The results are compared with experimental 2D-Angular Correlation of Annihilation Radiation (ACAR) and Coincidence Doppler Broadening Spectroscopy (CDBS) data.

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f Electron Behaviour in Rare Earth Based Systems: Localization or Itinerancy?

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Measurement of the two dimensional angular correlation of the electron-positron annihilation radiation (2D-ACAR) complemented with *ab-initio* calculations can provide decisive information about the *character* of the f-electrons in rare earth compounds. We provide examples of *f-electron localized* and *f-electron itinerant s*ystems, respectively. i) In the case of the antiferromagnetic heavy fermion and superconductor $CeIn_3$ the multisheet Fermi Surface (FS), reconstructed from our measurements in the paramagnetic phase, agrees closely with the predictions of band structure calculations regarding the Ce 4felectrons as fully localized. ii) On the other hand, our studies of the antiferromagnet actinide based UGa_3 in the paramagnetic phase, compared with calculations which include the effects due to the non uniform positron density and the electron-positron correlations, produce a substantial evidence that an unconstrained 5f-electron itinerant description applies.

Sensitivity of Positronium Momentum Distribution to Phase Transitions In Crystalline Dielectrics

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Positronium (Ps), a bound state of an electron and a positron, forms in various dielectric crystals[1]. Being a *light* impurity atom in a crystal lattice, Ps is extremely sensitive to its local surroundings and phonon lattice vibrations. In crystal lattices of non-cubic symmetry, the Ps atom may possess an effective quadrupole moment even in spite of the fact that it is completely electroneutral in vacuum [2]. In cubic crystal, Ps is neutral but interacts with phonons in a way different from that the electron does. Namely, the neutral Ps atom intensively interacts with short-range acoustic/optic deformation potentials only, not responding to long-range phonon-induced electric fields [3]. These two circumstances, the effective quadrupole interactions and short-range phonon interactions, make the Ps atom a tool for the study of symmetry-dependent structural properties of Ps-forming crystals. In particular, second order phase transitions in crystals, where the local symmetry of the lattice changes but the crystalline structure remains, may be sensed by a Ps momentum distribution measured in ACAR-experiments.

We give a review of the recent theoretical and experimental study of the Ps-phonon and Ps-quadrupole interactions in dielectric crystals of different local symmetries, making a special emphasis on the sensitivity of the Ps momentum distribution to the second order phase transitions in crystalline dielectrics.

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Positron Annihilation in Corroded Steels St20 and St3S

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The work deals with examining the lifetime of positrons emitted from ^{22}Na source in corroded St20 and St3S steels. Influence of the method of defecting the sample surface on the spectrum of positron lifetimes was investigated. Influence of temperature of initial annealing of samples, plastic deformation, type of corroding environment and electrolytic hydrogenation on trapping of positrons in the examined steels was also determined.