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SIXTH INTERNATIONAL CONFERENCE ON

POSITRON ANNIHILATION

The University of Texas at Arlington, April 3-7, 1982
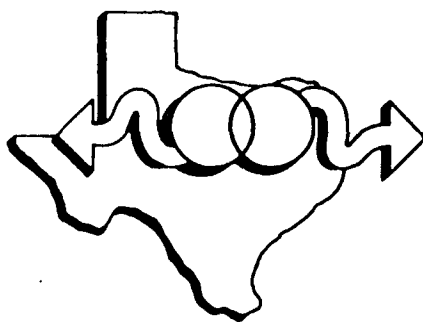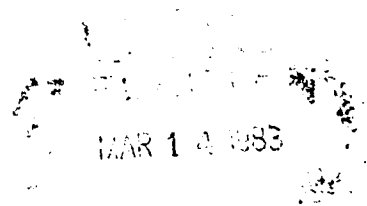
PROGRAM
AND
COLLECTED
ABSTRACTS

UTA

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Positron Annihilation

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See Over

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Low energy positron annihilation measurements have been used
widely in solid state physics, materials science, atomic and
molecular physics and chemistry, radiation chemistry, and medicine.
This Conference marked the fiftieth anniversary of the discovery
of the positron by Carl Anderson, and the Opening Address was
delivered by Professor Martin Deutsch of M.I.T., who discovered
positronium about thirty years ago. Thirty one invited papers
were presented covering all fields in which positron annihilation
is used. 270 contributed papers were presented in oral and poster
sessions. Of particular interest at this, the sixth conference
in this series, was the emergence of monoenergetic positron
beams as important tools in the study of fundamental processes
and of the surface properties of materials.
204 registrants from 22 countries attended the Conference.
59 selected scientists were awarded funds in partial support of
their participation in the Conference.
The Proceedings were published by North Holland in November, 1982.

SIXTH INTERNATIONAL CONFERENCE ON

POSITRON ANNIHILATION

The University of Texas at Arlington, April 3-7, 1982

PROGRAM
AND
COLLECTED
ABSTRACTS

UTA

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Our exhibitors have also made contributions to the Conference:

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PREFACE

Welcome to Texas! Our celebration of the fiftieth anniversary of the positron begins with the Opening Session at the University of Texas at Arlington on the afternoon of Saturday, April 3. We are honored to welcome Professor Martin Deutsch, who will present the keynote address, "Fifty Years of Positrons - Thirty Years of Positronium," at the Session.

The Program which is to be found at the beginning of this book differs slightly from the tentative program contained in the booklet mailed to prospective participants in February. Post-deadline papers have been moved to oral sessions or to the poster session, and a small number of papers have been transferred to different sessions, or withdrawn. Wherever possible, the numbering of papers in the program booklet has been retained.

The scientific sessions will be held at the Hyatt Regency Fort Worth. Invited papers will be presented in plenary sessions, and contributed papers will be presented orally in two parallel sessions and in a poster session. Titles of poster papers, which will be displayed during the entire Conference, are listed at the end of the program. The time allotted to contributed papers is either ten or twelve minutes, depending on the number of papers in the session. Thirty or forty minutes are allotted to each invited paper.

We should like to thank the members of the International Scientific Advisory Committee for their wise counsel, and all participants for their contributions, and we look forward to a Conference which will prove a worthy memorial to our colleague and friend John McNutt.
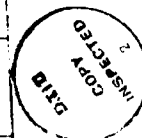
P. G. Coleman
S. C. Sharma
L. M. Diana

Arlington, February 22, 1982

CONTENTS

LIST OF INVITED PAPERS

OPENING SESSION

Time / Date

Date	a.m. 8:00 – 9:00	9:00 – 12:00	p.m. 12:00 – 1:00	1:00 – 3:00	3:00 – 4:00	4:00 – 5:30	6:00 – 8:00	8:00 – 10:00
Sat. April 3		REGISTRATION Hyatt Regency Fort Worth	Coaches to UTA	OPENING SESSION A1 Theater, UTA Address by Martin Deutsch	CHAMPAGNE RECEPTION / Return to Fort Worth	Return to Fort Worth	BARBEQUE Fort Worth Stockyards	RODEO Stockyards Coliseum
Sun. April 4	Breakfast	A GASES (Roellig, Stein, Schrader, Griffith) — Coffee	B Gases / C Metals	Lunch	D DEFECTS IN METALS (Siegel, Schaefer, Dupasquier, Hautojärvi)	Coffee — E Defects in Metals / F Non-metals	Dinner	P POSTER SESSION
Mon. April 5	Breakfast	G 2D ACAR (Singru, Manuel, Bansil) — Coffee	H 2D ACAR / J Techniques	Lunch	K POSITRON CHEMISTRY (Eldrup, Mogensen, Ache, Goldanskii)	Coffee — L Chemistry / M H,N,O in Metals	Dinner	N: Ps, ASTRO-PHYSICS, NONMETALS (Gidley, Drachman, Fujiwara, Brandt, Dekhtyar)
Tues. April 6	Breakfast	Q POSITRON TOMOGRAPHY (Derenzo, McKee, Mullani) — Coffee	R PET, Bio, Phase tran / S Al Alloys	Lunch	T SOLID STATE (Shiotani, Heinrich, Rozenfeld, Mackenzie)	Coffee — U Solid State / V Ps in Gases	Cocktail Party	BANQUET
Wed. April 7	Breakfast	W Pot-pourri / X Defects in Alloys — Coffee	Y SURFACES (Mills, Canter, Triftshäuser)	Z SUMMARY (Berko) / MA-RY — Lunch				

Sessions A,C,D,E,G,J,K,M,N,Q,S,T,U,W,Y,Z will be in section D of the Grand Crystal Ballroom. Sessions B,F,H,L,R,V,X will be in the Continental Room. Posters, exhibits and coffee will be in the Texas Ballroom. Breakfast, Lunch, and Dinner will be served in section C of the Grand Crystal Ballroom.

Saturday, April 3

REGISTRATION   9:00 a.m. - 12:00 noon, April 3, and throughout the Conference.

OPENING SESSION

Coaches leave the Hyatt Regency at 12:00 noon, April 3.
Session begins at 1:00 p.m. in the A-1 Theater on the campus of The University of Texas at Arlington.

Keynote Address:

"Fifty Years of Positrons: Thirty Years of Positronium"
MARTIN DEUTSCH

Champagne Reception 3:00 - 4:00 p.m.
Hosted by Dr. Wendell H. Nedderman, President of The University of Texas at Arlington.

Coaches leave for Fort Worth at 4:00 p.m.

BARBEQUE
6:00 p.m., Fort Worth Stockyards Coliseum.

RODEO
8:00 p.m., Fort Worth Stockyards Coliseum. The Coliseum was the site of the first ever indoor rodeo, in the year 1917.

Sunday, April 4

PLENARY SESSION A   9:00 - 10:45 a.m., Section D of the Grand Crystal Ballroom

> This Session is dedicated to the memory of John D. McNutt.

A-1   In Memoriam: John D. McNutt and Daniel R. Gustafson
      L. O. ROELLIG

A-2   Positron-Gas Scattering Experiments (Invited Paper, 30 mins.)
      T. S. STEIN and W. E. KAUPPILA

A-3   Bound States of Positronic Atoms and Molecules (Invited Paper, 30 mins.)
      D. M. SCHRADER

A-4   Positrons in Gases - A Progress Report (Invited Paper, 30 mins.)
      T. C. GRIFFITH

Coffee and Other Refreshments
10:45 - 11:05 a.m.
Texas Ballroom

E-6   Investigations of Vacancies in Ta in Thermal Equilibrium by Means of
       Positron Lifetime Measurements
       A. BALOGH, R. GUGELMEIER, and H.E. SCHAEFER

E-7   Positron Annihilation in the Plastic Zone at a Crack Tip
       JIANG JIAN, XIONG LIANGYUE, and LUNG CHI-WEI

E-8   Comparison between Studies of Lattice Defects by Positrons and Positive
       Muons
       MASAO DOYAMA

SESSION F   NON-METALS
             April 4, 4:05 - 5:30 p.m., Continental Room
             10 mins. for each paper.

F-1   Kinetics of Aggregation and Annealing of Defects in Heavily X-Irradiated
       Alkali Chloride Crystals Studied by Positron Annihilation
       STANLEY STERN and WERNER BRANDT

F-2   Positron Annihilation in Pb^{2+} Doped KCl Single Crystals
       M. CHINNUSAMY, S. RAMASAMY, T. NAGARAJAN, and V. MANOHAR

F-3   Annihilation of a Positron in a Vacancy in Graphite
       M. SHIMOTOMAI, T. TAKAHASHI, M. DOYAMA, and T. IWATA

F-4   Defects in Amorphous Silicon Films
       S. DANNEFAER

F-5   Positron Mobility in Germanium
       T. MCMULLEN

F-6   Temperature Dependence of the Time and Momentum Spectra in Germanium
       P. J. SCHULTZ and I. K. MACKENZIE

F-7   Three-Quantum Annihilation in Powdered Alumina
       C. DAUWE and MOTOKO KWETE

F-8   Enhancement Effect on Positron Annihilation in Solid Argon and Xenon
       B. K. SHARMA and HANUMAN SINGH

Dinner
Grand Crystal Ballroom, Section C

POSTER SESSION P   April 4, 7:30 - 9:30 p.m.
                        Texas Ballroom

Poster titles are listed at the end of the Program.

Monday, April 5

PLENARY SESSION G   2D ACAR
April 5, 9:00 - 10:45 a.m.
Section D of the Grand Crystal Ballroom

G-1   Two-Dimensional Angular Correlation: Theory and Experiment (Invited Paper, 45 mins.)
R. M. SINGRU

G-2   Progress in the Detection of Angular Correlation of Positron Annihilation using High Density Proportional Chambers (Invited Paper, 30 mins.)
A. A. MANUEL, R. SACHOT, P. DESCOUTS, and L. OBERLI

G-3   Electron and Positron States in Disordered Alloys (Invited Paper, 30 mins.)
A. BANSIL

Coffee and Other Refreshments
10:45 - 11:05 a.m.
Texas Ballroom

SESSION H   2D ACAR
April 5, 11:05 - 12:30, Continental Room
12 mins. for each paper.

H-1   Spin Dependent 2D ACAR Measurements in Gadolinium
K. R. HOFFMAN and S. BERKO

H-2   Studies of the Fermi Surface of Tantalum by 2D ACAR Measurements
F. SINCLAIR, K. R. HOFFMAN, and S. BERKO

H-3   The Autocorrelation Function $B^{+-}(r)$ in Positron Annihilation Physics
S. BERKO, W. S. FARMER, and F. SINCLAIR

H-4   Two-Dimensional Angular Correlation Studies of Defect and Defect-Related Problems in Metals
R. N. WEST

H-5   Two-Dimensional Electron-Positron Momentum Densities in the HCP Metals Mg, Zn, and Cd
P. A. WALTERS, J. MAYERS, and R. N. WEST

H-6   Two-Dimensional Angular Correlation of Annihilation Radiation from Neutron-Irradiated Aluminum
R. N. WEST, P. A. WALTERS, and J. D. MCGERVEY

H-7   2D Angular Correlation Experiments on αCuGe and αCuZn Alloys: The Reconstruction of Momentum Densities from Data
L. M. PECORA and A. C. EHRLICH

SESSION J   ADVANCES IN TECHNIQUES AND DATA ANALYSIS
April 5, 11:05 - 12:30. Section D, Grand Crystal Ballroom
10 mins. for each paper.

Lunch, 12:30 - 1:30 p.m.
Grand Crystal Ballroom, Section C

PLENARY SESSION K   POSITRON AND POSITRONIUM CHEMISTRY
                     April 5, 1:30 - 3:45 p.m.
                     Section D, Grand Crystal Ballroom

Coffee and Other Refreshments
3:45- 4:05 p.m.
Texas Ballroom

SESSION L   POSITRON AND POSITRONIUM CHEMISTRY
             April 5, 4:05 - 5:30 p.m., Continental Room.
             10 mins. for each paper.

L-1   Positronium Formation and Reactions in Water, Ice and Aqueous Solutions
       seen by Positron Age-Momentum Correlation
       Y. KISHIMOTO and S. TANIGAWA

L-2   The Temperature Dependence of Angular Correlation Curves for Solid
       Pivalic Acid
       P. C. JAIN, M. ELDRUP, O. E. MOGENSEN, D. LIGHTBODY, and J. N. SHERWOOD

L-3   Positron Annihilation Studies in p-Nitrobenzylidene-p-n-Alkyloxyanilenes
       P. C. JAIN and S.R.S. KAFLE

L-4   Positron Annihilation Studies in some Alkyl and Alkyoxy-Cynobiphenyls
       P. C. JAIN, S. R. S. KAFLE, V. G. BHIDE, and B. D. MALHOTRA

L-5   Re-Exam the Positron Lifetime on γ-Irradiated Ice Systems at 77K
       Y. C. JEAN, J. M. STADLBAUER, B. W. NG, and D. C. WALKER

L-6   Correlation between Pulse Radiolysis and Positron Annihilation Data
       J. CH. ABBÉ, G. DUPLÂTRE, A. G. MADDOCK, J. TALAMONI, and A. HAESSLER

L-7   Inhibition and Anti-Inhibition Effects Analyzed using Radiation Chemistry
       Data
       YASUO ITO, YASUHIRO MIYAKE, and YONEHO TABATA

L-8   Is the Positron a Light Proton? Proton-Positron Analogies
       P. E. CADE and C.M. KOW

SESSION M   H, N, AND O IN METALS
             IRRADIATED METALS
             April 5, 4:05 - 5:30 p.m. Section D, Grand Crystal Ballroom
             10 mins. for each paper.

M-1   Recovery of Deformed and Hydrogen-Charged Palladium
       C. L. SNEAD, JR., K. G. LYNN, and J. F. LYNCH

M-2   A Positron Study of Nitrogen Diffusion and Capture by Voids in Mo
       H. E. HANSEN, G. TRUMPY, and K. PETERSEN

M-3   The Interaction between Nitrogen and Defects in Mo Studied by the
       Positron Annihilation Technique
       B. NIELSEN, A. VAN VEEN, L. M. CASPERS, H. FILIUS, H. E. HANSEN, and
       K. PETERSEN

M-4   The Interaction between Hydrogen and Defects in Metals Studied by the
       Positron Annihilation Technique
       B. NIELSEN, A. VAN VEEN, L. M. CASPERS, W. LOURENS, G. TRUMPY, and
       K. PETERSEN

M-5   Temperature Dependence of Positron Annihilation Parameters in Neutron
       Irradiated Mo
       B. PAGH, H. E. HANSEN, B. NIELSEN, and K. PETERSEN

Coffee and Other Refreshments
10:45 - 11:05 a.m.
Texas Ballroom

SESSION R PET, BIOPHYSICS, PHASE TRANSITIONS
April 6, 11:05 - 12:30
Continental Room. 12 mins. for each paper.

R-1 The High-Density Avalanche Chamber for Positron Imaging
A. JEAVONS, R. CLACK, A. DONATH, P. FREY, G. HERLIN, K. HOOD, R. MAGNANI,
D. TOWNSEND

R-2 Positron Annihilation in Erythrocyte Membrane
S.Y. CHUANG, M.E. OTTLINGER, and M.F. LOU

R-3 Positron Studies of Phase Transitions of Phospholipids
Y.C. JEAN

R-4 Positron Annihilation Studies of Phase Transitions of Ferroelectric,
Ferromagnetic, and Antiferromagnetic Crystals
F. H. HSU, H. S. LIU, and E. R. VANCE

R-5 The Measurements of the Doppler Broadening of Positron Annihilation due to
the CDW Phase Transformations in $1T-TaS_2$
A. SUZUKI, T. HATANO, R. YAMAMOTO, M. DOYAMA, K. ENDO, H. IHARA, and
S. GONDA

R-6 Positron Lifetime and Doppler Broadened Line Shape Parameters in Chevrel
Phase Compounds
V. MANOHAR, S. RAMASAMY, T. NAGARAJAN, C.S. SUNDAR, K.P. GOPINATHAN,
A.M. UMARJI, and G.V. SUBBA RAO

R-7 Positron Annihilation Parameters Close to the Melting Point and at Phase
Transitions
P. SPERR, QUIN MIN FAN, and W. TRIFTSHÄUSER

SESSION S ALUMINUM ALLOYS
April 6, 11:05 - 12:30
Section D, Grand Crystal Ballroom. 10 mins. for each paper.

S-1 The Precipitation Mechanism of Ge in Al Studied by Positron Annihilation
H. MURAKAMI, I. KANAZAWA, T. KURIHARA, T. SHIMIZU and M. DOYAMA

S-2 The Recovery of Quenched Al-Sn Alloys Studied by Positron Annihilation
I. KANAZAWA, M. MURAKAMI, T. KUSUKA, Y. SAKURAI, and M. DOYAMA

S-3 Positron Annihilation in Al-0.55 at .% Mn
T. TROEV and P. TOPALOV

S-4 Positron Studies of Solute Clustering and Lattice Defects in Al-Zn Alloys
A. ALAM and R.N. WEST

                        Lunch, 12:30 - 1:30 p.m.
                  Grand Crystal Ballroom, Section C

PLENARY SESSION T   SOLID STATE
                    April 6, 1:30 - 3:45 p.m.
                    Section D, Grand Crystal Ballroom

      This Session is dedicated to the memory of Daniel R. Gustafson

                     Coffee and Other Refreshments
                          3:45 - 4:05 p.m.
                          Texas Ballroom

SESSION U   AMORPHOUS AND OTHER ALLOYS: SOLID STATE
            April 6, 4:05 - 5:30 p.m.
            Section D, Grand Crystal Ballroom. 10 mins. for each paper.

Cocktail Party
7:00 - 8:00 p.m.
Grand Crystal Ballroom

BANQUET
8:00 p.m.
Grand Crystal Ballroom

Wednesday, April 7

SESSION W POTPOURRI
April 7, 9:00 - 10:25 a.m.
Section D, Grand Crystal Ballroom. 10 minutes for each paper.

W-1 Observation of the $1^3S_1 - 2^3S_1$ Energy Splitting in Positronium
A.P. MILLS, JR. and S. CHU

W-2 Evidence of Excited State Ps Formation from a Clean Metal Surface in Ultra-High Vacuum
D. SCHOEPF, S. BERKO, K.F. CANTER, A. WEISS

W-3 Exact First Order Electron Self-Energy Contribution to the Decay Rate of Positronium
MICHAEL A. STROSCIO

W-4 Do Positron Lifetimes Reflect the Age of the Universe?
J.T. MUHEIM

W-5 A Model for the Shelf in the Diffuse γ-Ray Spectrum
RICHARD L. LIBOFF and DANIEL M. HEFFERNAN

W-6 Single-Positron Analysis for the Study of Transient Electronic Processes in Insulators
L. YARMUS, V.P. SHANTAROVICH, and WERNER BRANDT

W-7 Positron Annihilation in Heterogeneous Substances
V.P. SHANTAROVICH, L.G. ARAVIN, V.A. ONISCHUK, B.M. LEVIN, and V.I. GOLDANSKII

W-8 Positron Energy Loss Measurements in Thin Silicon and Polycrystalline Carbon Foils
K. G. LYNN, W. FRIEZE, and D. FISCHER

SESSION X DEFECTS IN ALLOYS
April 7, 9:00 - 10:25 a.m.
Continental Room. 12 minutes for each paper.

X-1 Study of Vacancy-Solute Interactions in Dilute Lead Based Alloys by Thermal Equilibrium Measurements of Annihilation Lineshapes
K. ITO, Y. OHTSU, and S. TANIGAWA

X-2 Transferred to Poster Session

Coffee and Other Refreshments
10:25 - 10:45 a.m.
Texas Ballroom

PLENARY SESSION Y   SURFACES
                    April 7, 10:45 - 12:30
                    Section D, Grand Crystal Ballroom

PLENARY SESSION Z   April 7, 12:30 - 1:00 p.m.
                    Section D, Grand Crystal Ballroom

       Summary of the Conference
       S. BERKO

Lunch
1:00 - 2:00 p.m.
Grand Crystal Ballroom, Section C

POSTER SESSION P   April 4, 7:30 - 9:30 p.m.
                   Sections B and C, Texas Ballroom
                   Posters will remain in place throughout the Conference.

     Beer and other refreshments will be available on the evening of April 4
     to encourage an informal atmosphere.

METALS

P-1   Possible Positron-Lattice Interaction at Elevated Temperatures of Cadmium
      W.F. HUANG and L.D. BURTON

P-2   Enhancement Factors of the Annihilation Rates of Umklapp Terms in Metals
      H. SORMANN, P. NOWAK, P. KINDL, and W. PUFF

P-3   Positron Lifetime Measurements in Indium
      W. PUFF, P. MASCHER, P. KINDL, H. SORMANN

P-4   Positron Annihilation, Mossbauer Effect, and X-Ray Diffraction Studies of
      Electrodeposited Ni
      A. VÉRTES, ZS. KAJCSOS, I. CZAKÓ-NAGY, M. LAKATOS-VARSÁNYI, H. LEIDHEISER,
      JR.

P-5   Influence of an Exchange Correction on Lifetime and Enhancement Factor in
      kahana's Formalism
      Z. SZOTEK

P-6   Positron Annihilation in Zinc
      Z. PAWLOWSKA

P-7   APW Calculation of the Positron Angular Correlation in PD and PDH
      A. HARMALKAR, D.G. KANHERE, R.M. SINGRU

P-8   Positron Annihilation in Single Crystals of Palladium- and Tantalum-
      Hydrides
      M. HASEGAWA, H. ASANO, and M. HIRABAYASHI

P-9   Momentum Density for Positron Annihilation in Rhodium
      S.B. SHRIVASTAVA and H.P. BONDE

P-10 Investigation of Momentum and Spin Density of Ferromagnetic Nickel and
      Iron by Positron Annihilation
      W. GERBER, G. DLUBEK, and O. BRÜMMER

P-11 The Prevacancy Effects in Metals Observed by Positron Annihilation
      LARS C. SMEDSKJAER

P-12 Positron Lifetimes in γ- and α- Cerium
      J.D. MCGERVEY, S.G. USMAR, N. PANIGRAHI, and C.Y. HUANG

ADVANCES IN TECHNIQUES AND DATA ANALYSIS

xxx

P-153   Positrons in Biomolecular Systems II
        GEORGE GRAF and JAMES C. GLASS

POSTDEADLINE PAPERS   may be presented as posters, beginning with P-154.

EXHIBITION
There will be an exhibition of equipment in the Texas Ballroom throughout
the Conference. The exhibitors are:

> Air Products and Chemicals, Inc.
> Alphatronix S.A. (Geneva)
> Bicron Corp.
> E. G. & G. Ortec
> Hamamatsu Corp.
> New England Nuclear Corp.
> Nuclear Data, Inc.

ABSTRACTS

Keynote Address
The Opening Session of the Sixth International Conference
on
Positron Annihilation

The University of Texas at Arlington
April 3, 1982

FIFTY YEARS OF POSITRONS:
THIRTY YEARS OF POSITRONIUM

MARTIN DEUTSCH

Massachusetts Institute of Technology
Cambridge, MA 02138, U.S.A.

IN MEMORIAM
JOHN D. MCNUTT AND DANIEL F. GUSTAFSON

L. O. Roellig
C.U.N.Y., 535 E. 80 St., New York, NY 10021, U.S.A.

POSITRON-GAS SCATTERING EXPERIMENTS*

T. S. Stein and W. E. Kauppila
Department of Physics and Astronomy
Wayne State University, Detroit, Michigan 48202, U.S.A.

During the first decade of positron-gas scattering experiments, total scattering cross sections have been measured for the inert gases and for a variety of molecules by several different groups. These measurements have resulted in observations of some interesting qualitative features including Ramsauer-Townsend effects in He and Ne (and possibly a shallow Ramsauer-Townsend minimum in Ar), abrupt increases in the total cross sections of the inert gases and several different molecules near the predicted thresholds for positronium formation, and a merging of the e^+ and e^--He total cross sections at a much lower energy (~ 200 eV) than was expected. Experimental positron-gas scattering areas beyond total cross sections, such as differential cross sections, elastic, excitation, ionization, and positronium formation cross sections, and searches for resonances (temporary bound states) are in very early stages of exploration. Our main goals in this progress report are to (1) discuss what we feel are the most significant developments in the first decade of positron-gas scattering experiments, (2) point out some consistent patterns in the experimental results in cases where several different groups have investigated the same collision processes, and (3) present some puzzling questions raised by the new generation of experiments which go beyond total cross section measurements. The differences and similarities between the observed scattering behavior of positrons and electrons will be emphasized.

BOUND STATES OF POSITRONIC ATOMS AND MOLECULES

D. M. Schrader

Chemistry Dept., Marquette Univ., Milwaukee, WI 53233, USA

A complete discussion of positron-atom and -molecule interactions includes scattering states, but these have been reviewed recently by the author[1] and will not be considered here. We concern ourselves here with chemical stability of systems which contain at least one each of: positrons, electrons, and nuclei. The chemical stability of such systems can be defined as follows:

Such a system may be said to be chemically stable if it does not spontaneously rearrange itself into separated parts before it annihilates. According to this definition a system is necessarily chemically stable if, ignoring coupling to the radiation field, the total energy of the system is below the onset of the lowest continuum. But this is not the only way that chemical stability may manifest itself. In any case, chemical stability can, in principle, be demonstrated either by laboratory experiments or by calculations. In fact, the existence of a bound state of only one positron-electron-nuclear system has been proven, and that by calculations. The system is positronium hydride, PsH[2]. Less rigorous but nevertheless thoroughly convincing evidence indicates the chemical stability of the lighter positronium halides[3, 4] as well as positronium nitrate[5] and several positronic diatomic molecules[6]. All this evidence is from quantum chemical calculations. The experimentalists have contributed virtually nothing to the question of chemical stability. It is strange and remarkable that in our field, we do not know the energies of most of the systems with which we work, or even whether bound states of them exist. Such a state of ignorance would be regarded as appalling in most other areas of chemistry and physics.

In the present review, the quantum chemical methods which have been applied to mixed positron-electron systems are reviewed. These include methods which provide an upper bound to the total energy (Hylleraasian expansions, several variants of Hartree-Fock self-consistent field formulations, and extensions to configuration interaction methods), and those which do not (various adiabatic-like models, methods which involve empirical model potentials, and semiempirical molecular orbital methods).

The results of applications of these methods are then initially reviewed. Special attention is given to the calculation of annihilation rates and angular correlation curves.

Finally, the extremely sparse and indirect contributions from experiment to the question of chemical stability are considered.

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POSITRONS IN GASES- A PROGRESS REPORT

T.C.Griffith

Department of Physics and Astronomy, University College London

Gower Street, London, WC1E 6BT.

In this short review an account will be given of the recent work done at University College and, where relevant, a comparison will be made with similar work performed by other groups. Three groups of experiments will be discussed:-

(1) Lifetime studies. Several new and noteworthy features (relating to Z_{eff} and positronium fractions) in the lifetime spectra of positrons in various gases were recently reported by Heyland et al[1]. Further investigations of these features for other gases and for mixtures of gases will be reported and some of the possible mechanisms needed for interpretation of the data will be discussed.

(2) Direct measurement of positronium formation cross-section. Relative values of these cross-sections as a function of energy were reported by Charlton et al[2]. Modifications of the earlier system used for this work should enable determination of absolute cross-sections and it is hoped that preliminary results for a number of gases can be presented.

(3) The total cross-sections for positrons and electrons scattered in various gases have been re-measured using improved experimental techniques and refined methods of analysis. Some of the recent results will be briefly reported.

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TOTAL CROSS-SECTIONS FOR POSITRON SCATTERING IN NITROGEN AT ENERGIES FROM 20 to 3000 eV

J. Dutton, C. J. Evans and H. L. Mansour

Department of Physics, University College of Swansea, University of Wales, Swansea, U. K.

The total scattering cross-section of positrons in nitrogen has been measured over the energy range 20 to 3000 eV.   There are no previously published results from other groups over the range 800 - 3000 eV (either for positrons or electrons) which can be used for comparison but the results below 800 eV show good agreement with previously published data[1].

These results were obtained using a scattering chamber based on a 180° magnetic spectrometer[2] with a retarding-field energy-analyser, followed by a detector of coincident annihilation radiation.   A 2 mCi ^{22}Na source was used with an MgO moderator as the source of slow positrons, and this necessitated counting times of the order of 24 hours in order to reduce the statistical error to a value comparable with other sources of error.   Possible sources of systematic error have also been considered and shown to contribute a negligible proportion of the total error, which is itself less than 5% over the energy range 75 - 2750 eV.

In the absence of other experimental results at energies above 800 eV, it was of interest to use the Bethe-Born theory as reviewed by Inokuti[3] to assess the validity of the present data in this region.   On the basis of this theory it can be shown that the results lead to a value of 4.8 $\pm$ 0.2 for the sum-of-dipole-moments-squared M_{tot}^2. This compares with a value of 4.7 calculated from data on optical absorption and electron scattering[4] and a value of 5.0 obtained from measurements of magnetic susceptibility[5].

The agreement obtained validates the experimental method over the high energy range and incidentally provides a new and independent measurement of the quantity M_{tot}^2.

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ELASTIC SCATTERING OF POSITRONS BY ATOMIC
HYDROGEN AT INTERMEDIATE ENERGIES

R.S.Pundir and K.C.Mathur

Department of Physics, University of Roorkee, Roorkee 247672,India

The elastic scattering of positrons by atomic hydrogen H(1s) is studied in the frame-work of the two potential method at intermediate energies. The T-matrix is given by[1]

$$T = \langle \psi_f | U | \chi_i^{(+)} \rangle + \langle \chi_f^{(-)} | W | \chi_i^{(+)} \rangle$$

where $U = \zeta(r_2)/r_2$ and $W = -1/r_{12} + (1-\zeta(r_2))/r_2$. $\vec{r}_1$ and $\vec{r}_2$ are the position vectors of atomic and incident particles. $\zeta(r_2)$ is a position dependent screening parameter and $\psi_f(\vec{r}_1,\vec{r}_2) = \mathrm{Exp}(i\vec{k}_f \cdot \vec{r}_2) U_f(\vec{r}_1)$, where $U_f(\vec{r}_1)$ is the final state atomic wave function.

Considering polarisation we express

$$\chi_i^{(+)}(\vec{r}_1,\vec{r}_2) = F_i^{(+)}(\vec{r}_2)\left\{U_i(\vec{r}_1) + U_{Pol}(\vec{r}_1,\vec{r}_2)\right\}$$

U_{pol} is the polarisation term[3]. The distorted waves $F_n(\vec{r}_2)$ in the initial and final channels are obtained from the following Eq.

$$\left\{(1/2)\nabla_2^2 - \zeta(r_2)/r_2 + (1/2)k_n^2\right\} F_n(\vec{r}_2) = 0 \, ,$$

subject to the usual boundary conditions.

The differential cross section is given by

$$\frac{d\sigma}{d\Omega} = \frac{k_f}{k_i}\frac{1}{4\pi^2}|T|^2$$

Figure shows our result for $e^+ + H(1s)$ elastic differential cross section at 400 eV energy. We find that for angles greater than 10° our results are in reasonable agreement with the recent calculation of Byron and Joachain[4](BJ) based on the third order optical potential method. For lower angles we obtain a dip in the cross section due to the interference between static and polarisation contributions. Further results will be presented at the time of conference.

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ANNIHILATION PARAMETER FOR POSITRON MOLECULE COLLISIONS
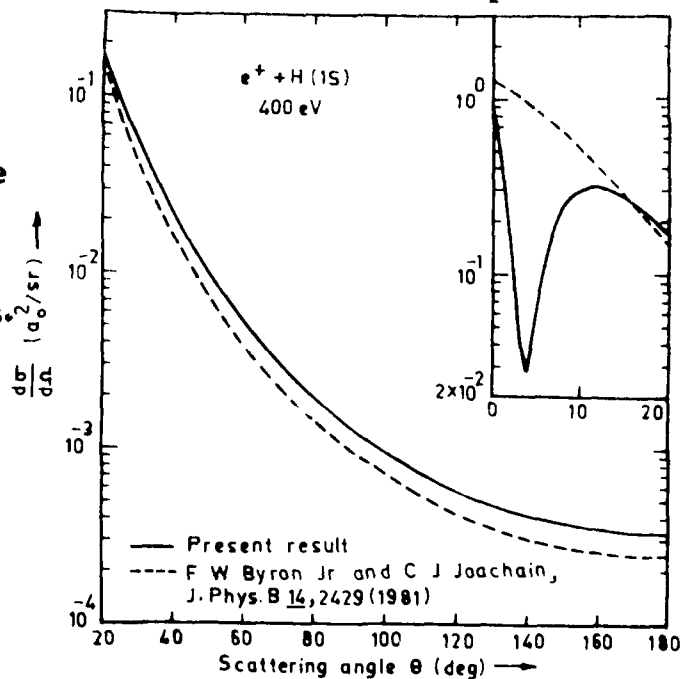
Sukannya Sur and A.S.Ghosh
Department of Theoretical Physics, Indian Association for the
Cultivation of Science, Calcutta 700032, India.

In the present study, we are calculating the annihilation parameter Z_{eff} for e^+-H_2 collisions in the low energy region. In our earlier paper[1] we have studied the elastic scattering of slow positrons by hydrogen molecules following the method of Hara[2] .

The annihilation parameter, Z_{eff}, is obtained from the relation

$$Z_{eff} = \sum_{i=1} \int |F(\overline{r})|^2 \rho(\overline{r}_i) d\tau \qquad (1)$$

Here $\rho(\overline{r}_i)$ is the charge density of the ith bound electron. We have expressed $F(\overline{r})$, the wave function of the incident positron in the following way,

$$F(\overline{r}) = \sum_L (2L+1)^{1/2} \frac{u_{Lo}(r)}{r} Y_{Lo}(\hat{r}) \qquad (2)$$

Where $u_{Lo}(r)$ satisfies the following equation

$$\left[\frac{d^2}{dr^2} - \frac{L(L+1)}{r^2} - 2V_o(r) - \frac{2L(L+1)}{(2L-1)(2L+3)} V_2(r) P_2(\hat{r}.\hat{R}) + k_o^2 \right] u_{Lo}(r) = 0 \qquad (3)$$

Our results are presented in fig.1 in the energy range 0.136 eV to 13.6 eV. Our results appreciably differ from those of Lodge et al[3] and Hara[4] quantitatively, our values being higher. The feature of our curve is similar to that of helium atom except at very low energies. The feature in the energy region $k_o < 0.05$ has not been noticed in the case of helium. We believe this to be the characteristics of a diatomic molecule for which the electron density is different from that of the corresponding atomic case.

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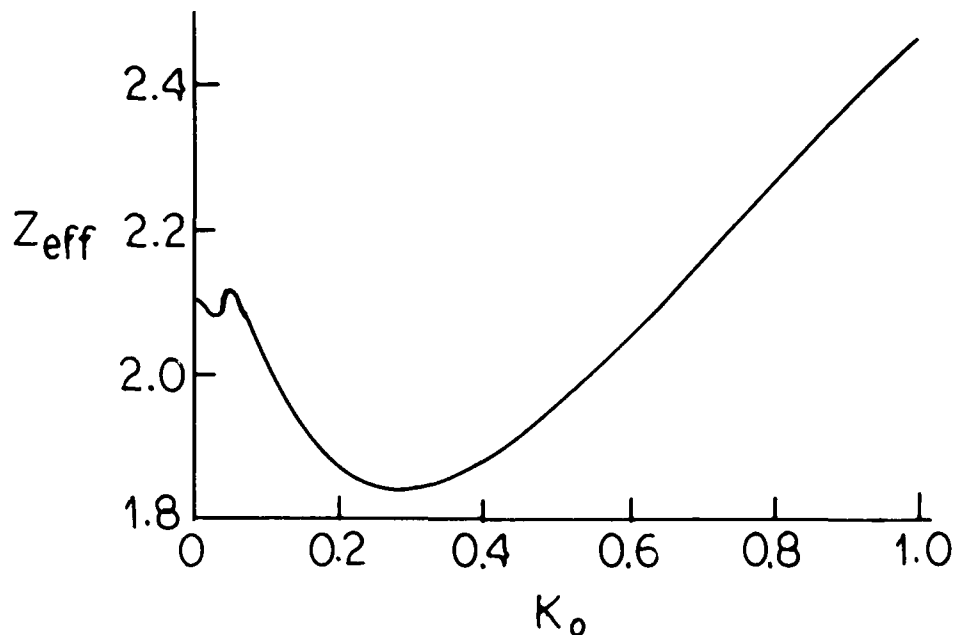
EFFECT OF CUT-OFF PARAMETER ON
LOW ENERGY POSITRON SCATTERING BY THE N_2 MOLECULE

A.K.Pande and R.S.Singh
Physics Department, Banaras Hindu University
Varanasi-221005, INDIA

The aim of this paper is to present a systematic effect of cut-off parameter on rotational excitation cross section for the positron scattering by the nitrogen molecule in the low energy region (.0136ev to ? ev). We have taken three values of the cut-off parameter i.e. $1.7 a_0$, ? and ? as used by the previous workers[1,2]. It means that any value of the cut-off parameter can not be used for all the energies. However, the whole energy range may be divided into two ? parts ? cut-off parameter point of view. ? ? on the basis of experimental values[3,4] ? ? the study gives us a prescription for ? ? suitable value of the cut-off parameter for the study of rotational excitation and inelastic scattering cross section in the positron ? scattering by the nitrogen molecule.

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POSITRON ANNIHILATION IN NITROGEN

K. Rytsölä, K. Rantapuska, P. Hautojärvi
Laboratory of Physics, Helsinki University of Technology
SF-02150 Espoo 15, Finland

Positron lifetime in nitrogen has been measured at temperature 67...390 K and at pressures up to 70 bar. At high temperatures the annihilation rate is known to vary slightly nonlinearly with density so that the effective electron number Z_{eff} seen by the positron decreases from about 30 at low densities to about 20 at 200 amagats /1/. At low temperatures, both above and below the critical point of the bulk liquid (126.2 K), relatively abrupt and strong deviations from this normal dependence are observed indicating a clustering phenomenon analogous to that seen in low temperature helium /2/. The behaviour of the annihilation rate as a function of density resembles closely that in hydrogen at 77 K and in methane at room temperature /3,4/. At a given density the increase in Z_{eff} is roughly by a factor of 10 at low temperatures (compared to that measured at 300 K) decreasing smoothly with temperature so that above about 250 K only small effects are seen. Thus the critical temperature for the clustering is about twice the normal critical temperature as in the case of helium. Even at high temperatures the annihilation rate decreases with temperature but this effect can be seen at all densities and is evidently not connected with clustering.

Theoretical calculations with the density functional method have been made of the cluster around the positron in low temperature nitrogen. The experimental behaviour of the annihilation rate versus density is well reproduced by the theory. In particular the softness of the transition to the cluster state is brought about by including the Bolzmann factor. On the basis of the calculations the e^+-N scattering length can be estimated to be $-2a_o...-3a_o$.

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LOW-ENERGY POSITRON AND POSITRONIUM ANNIHILATION IN ETHANE GAS

S.C. Sharma, A. Eftekhari, J.S. Hart, P.G. Coleman, L.M. Diana
Center for Positron Studies, Box 19059, UTA Station
The University of Texas at Arlington, Arlington, Texas 76019, U.S.A.

Positronium formation fractions and the annihilation rates of o-Ps and free positrons have been measured in gaseous ethane at several temperatures between 256 and 378K for densities in the range 1.2 - 286 amagat. The observed dependencies of the o-Ps annihilation rates on density and temperature of the gas can be interpreted in terms of density fluctuations in ethane. The Ps yields exhibit a strong dependence on density and appear to be independent of temperature between 256-378K. The annihilation rates of low-energy positrons indicate the formation of positron-ethane collision complexes and self-trapping of positrons in clusters of gas molecules.

COMPARISONS OF POSITRON ANNIHILATION
PARAMETERS IN n-NONANE AND SOME
OF ITS ISOMERS AT SIMILAR DENSITIES

S.R. Tuttle, L.M. Diana, S.C. Sharma, P.G. Coleman,
S.Y. Chuang, D.R. Barker, and J.N. McKamy
Center for Positron Studies, Box 19059, UTA Station
The University of Texas at Arlington, Arlington, Texas 76019, U.S.A.

Positron lifetimes and intensities were measured in degassed 99% pure n-nonane,2,2,4,4-tetramethylpentane, and 3,3-diethylpentane at several approximately equal densities. Comparisons of the results for the three liquids will be discussed.

POSITRON ANNIHILATION IN ORIENTED CRYSTALS
OF CADMIUM AND ZINC AS A FUNCTION OF TEMPERATURE

P. Rice-Evans, I. Chaglar and A.A. Berry
Department of Physics, Bedford College, University of London,
Regent's Park, London, NW1 4NS, England.
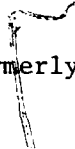
Measurements of Doppler Broadening of Radiation resulting from the Annihilation
of Positrons in single crystals of zinc and cadmium have been made as a function
of orientation and temperature.   Anisotropy in the observed characteristics is
discussed.

MOMENTUM DEPENDENT ANNIHILATION RATE FOR POSITRONS IN METALS

D. Neilson*
School of Physics, University of New South Wales,
Kensington, Sydney, N.S.W. 2033. Australia.

Results are presented of a calculation for the partial annihilation rate
of a thermalised positron with electrons in a metal as a function of the
initial electron momentum. The method used has previously been successfully
applied to the calculation of total annihilation rates. Recent work has
shown that the agreement with experimental total rates is even better than
was originally claimed. In this method the positron electron wave function
is calculated self-consistently using an effective interaction which
includes strong interaction effects from no more than one highly correlated
screening electron at any instant of time. Within the formalism self energy
insertions must be retained. The partial rates are more sensitive to these
insertions than are the total rates. The calculated partial annihilation
rates in the electron gas at metallic densities are all monotonically
increasing functions of the initial electron momentum up to the Fermi
surface. For Lithium the partial rate is in good agreement with experimental
data.

* Formerly D.N. Lowy

VARIABLE ENERGY POSITRON STUDIES IN WELL-ANNEALED
SINGLE CRYSTAL Cd SAMPLES FROM 50 TO 450 K

K. G. Lynn, A. N. Goland, P. Schultz, and A. Vehanen
Brookhaven National Laboratory*
Physics Department
Upton, New York   11973, U.S.A.

I. K. MacKenzie
University of Guelph
Physics Department
Guelph, Ontario N1G 2W1, Canada

Well-annealed Cd(001) and Cd(100) samples have been examined using a monoenergetic variable-energy positron beam (0.5 to 5.0 keV). The results are interpreted in the context of a one-dimensional-diffusion model which allows for annihilations as well as trapping at defects including thermally generated vacancies. The dependence on temperature of positron diffusion out of these samples was determined by the use of this model to interpret data taken between 50 and 450 K. The deduced positron diffusion length is in rough agreement with positron-acoustic-phonon scattering predictions[1] between 50 and 320 K (i.e., before onset of positron-vacancy trapping). No indication of positron localization in shallow traps is inferred from these results. These conclusions are consistent with our previous suggestion[2] that positron dynamics in well-annealed high-purity Cd single crystals are dominated by the intrinsic properties of the metal.

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IMPORTANCE OF ELECTRON-ELECTRON CORRELATIONS FOR POSITRON ANNIHILATION IN AN ELECTRON GAS ON THE BASIS OF A SIMPLE MODEL

H. Stachowiak
Institute for Low Temperature and Structure Research,
Polish Academy of Sciences,
Pl. Katedralny 1, 50-950 Wrocław, Poland

A model of electron-positron interaction in an electron gas is presented having some features similar to the Kahana approach[1]. Its simplicity allows to reach self-consistency easily (of course, within the model). Two variants of the model are investigated: the first one neglecting electron--electron correlations like in the original Kahana approach, the second taking them into account like Arponen and Pajanne did[2,3]. The variation with electron density of the positron lifetime and momentum dependent enhancement factor in each of these cases is similar to the behaviour of the same quantities according to Kahana on one side and Arponen-Pajanne on the other. This suggests that neglecting electron-electron correlations is an essential reason of the difficulties encountered in the Kahana approach, while the other objections against using the Bethe-Goldstone equation that can be found in the literature seem to be of lesser importance.

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MANY BODY INTERACTIONS OF POSITRONS IN POTASSIUM

T. Hyodo, T. McMullen* and A.T. Stewart
Department of Physics, Queen's University
Kingston, Ontario, Canada K7L 3N6

A series of experiments is in progress aimed at obtaining accurate observation of positron dynamics in potassium. If the temperature dependance of the positron momentum distribution is measured with sufficient accuracy, it may be possible to separate the positron-electron and positron-phonon many body effects.

Preliminary data at 79K show that a Gaussian momentum distribution of positron fits the observed Fermi cut-off smearing if the positron apparent mass is taken to be 1.2 ± 0.15.

An attempt will be made to separate the two different effects after data at a few different temperatures are accumulated.

* Present address: Department of Physics, Memorial University,
                   St. Johns, Newfoundland, Canada

POSITRON MOTION IN METALS: THERMAL SMEARING OF THE MOMENTUM DISTRIBUTION

T. McMullen
Physics Department, Memorial University of Newfoundland
St. John's, Newfoundland A1B 3X7
and
T. Hyodo and A. T. Stewart
Physics Department, Queen's University
Kingston, Ontario, Canada

The theory of thermal smearing of the Fermi cutoff in position angular correlation spectra of metals is due to Mikeska[1] and to Bergersen and Pajanne[2]. The important effect is a lifetime broadening caused by positron-phonon scattering. The positron momentum distribution resulting from this scattering is well described by a Gaussian distribution $\exp(-p^2/2m^{**}k_BT)$, but the "mass" which enters is not the positron effective mass m^* as conventionally defined[1] but an "apparent" effective mass m^{**}. We have found an analytic expression for the temperature dependence of $m^{**}(T)$ by using the positron spectral function resulting from positron-acoustic phonon scattering in metals. The result is

$$\frac{m^{**}(T)}{m^*} = 1 + 0.64\ \tilde{\chi}\ \left(\frac{m^*}{m_b}\right)^{3/2} \sqrt{\frac{T}{T_F}}$$

where $\tilde{\chi}$ is the positron-phonon coupling constant, and m^* the conventional effective mass including band, positron-electron, and the negligibly small positron-phonon mass renormalization. m_b is the positron band mass. This result implies that a plot of experimental data for $m^{**}(T)$ vs $\sqrt{T}$ extrapolates to the conventional effective mass m^*, giving an experimental value which can be compared with theories of the positron-electron mass enhancement. The slope gives the positron-phonon coupling. The m^{**} value obtained from a direct fit in long slit geometry is given by a similar formula, but with a different numerical coefficient.

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POSITRON ANNIHILATION CHARACTERISTICS IN REAL METALS INCLUDING MANY-BODY
ENHANCEMENT: A DENSITY-FUNCTIONAL APPROACH*

B. Chakraborty

Materials Science Division, Argonne National Laboratory,
Argonne, Illinois 60439, U.S.A.

A formalism has been developed for incorporating electron-positron
correlation effects into band-structure calculations of annihilation
characteristics. A two-component density-functional scheme is used, within the
local density approximation. The electron-positron correlation energy for an
interacting electron gas is taken from the work of Arponen and Pajanne[1]. A
generalization of the Kohn-Sham scheme is used to determine the electron and
positron densities self-consistently, with the electron-positron correlation
effects acting as an effective potential analogous to the electron-electron
exchange and correlation potentials. To determine the lifetime and angular
correlation spectra, a knowledge of these quantities in an interacting electron
gas is needed as a function of electron density. These were also obtained from
Ref. 1. The method was applied to aluminum as a test case, since extensive
experimental and theoretical information is available for this metal. The
calculated bulk positron lifetime (165 ps) is in excellent agreement with the
experimental value. The calculated two-dimensional angular correlation spectra
have been compared to experiment[2] and found to be in very good agreement. The
present theoretical results will be compared to earlier independent-particle-
model calculations to demonstrate the enhancement effects. The relative
enhancements of core and valence electrons will also be discussed.

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Institute of Metals, Sendai 1979).

"Positron Oscillations in Metals"

by

M.P. SRIVASTAVA
Department of Physics and Astrophysics
University of Delhi, Delhi-110007, India.

Abstract :

The behaviour of positrons in metals have been studied by many
workers with the aim of studying lifetime, angular Correlation etc.
In a simple metal, however, there are free electrons which are moving
rapidly in the lattice and give rise to conduction current in a metal.
If there is a swarm of positrons in the metal, the overall change
neutrality is broken for the system. Such change densities due to
positrons will set up electric fields which in turn will be responsible
for the motion of positrons. The consistent set of equation for the
distribution function of positrons is set up in conjunction with an
equation for electric field. It is found that such a system will have
a natural frequency of positron Oscillation. Such high frequency
Oscillations may be observed depending on the lifetime of annibilation
being large compared to the period of Oscillation.

POSITRON ANNIHILATION SPECTROSCOPY OF DEFECTS IN METALS:
A CRITICAL ASSESSMENT AND COMPARISON WITH OTHER TECHNIQUES[*]

R. W. Siegel
Materials Science Division, Argonne National Laboratory
Argonne, Illinois 60439, U.S.A.

The application of positron annihilation spectroscopy (PAS) to the characterization and study of defects in metals has grown rapidly and increasingly useful in recent years. Owing to the ability of the positron to annihilate from a variety of defect-trapped states in metals, PAS can yield defect-specific information which, by itself or in conjunction with other, more traditional experimental techniques, has already made significant contributions to our knowledge regarding lattice-defect properties in metals. These contributions have been primarily in two areas: (i) the determination of atomic defect properties, especially those of vacancies, and (ii) the monitoring and characterization of microstructure development, for example, during post-irradiation annealing. The application of PAS to the study of defects in metals will be reviewed and the results compared with those from other available techniques. An evaluation will be made of the strengths, and weaknesses, of PAS as a method for the characterization of defect microstructures vis-à-vis some of the other tools of the materials scientist. The further possibilities for using the positron as a localized probe of the structures of atomic defects will be discussed in terms of both the theoretically expected annihilation characteristics of a defect-trapped positron and experimental observations. Finally, an assessment of the present status of PAS as a tool for the study of defects in metals will be presented, and its future potential relative to other techniques will be considered.

EQUILIBRIUM DEFECTS IN METALS

H.E.Schaefer

Institut für Theoretische und Angewandte Physik
der Universität Stuttgart,7 Stuttgart 80,W-Germany

A review of the investigations of vacancy formation in thermal
equilibrium in the fcc and bcc metals by means of positron annihila-
tion will be given.A comparison of vacancy formation data with the
results of self-diffusion measurements will be presented in order to
discuss non-equilibrium experiments yielding data on vacancy migra-
tion.

Particular emphasis will be given to recent positron lifetime
measurements in thermal equilibrium on high melting transition me-
tals.The results of a detailed analysis of the lifetime spectra will
be presented and discussed in terms of present trapping models.

POSITRON LIFETIMES IN PRESENCE OF A
NON-UNIFORM DISTRIBUTION OF TRAPS

A. Dupasquier
Istituto di Fisica del Politecnico, Milano, Italy, and
Gruppo Nazionale di Struttura della Materia del CNR, Italy

Most experiments on positron annihilation in solids containing lattice defects are interpreted on the basis of the simplest well--known version of the trapping model, mathematically described by a set of differential equations with time- and position-independent coefficients. However, when the trap distribution is non-uniform over regions more extended than a fraction of the average diffusion length of thermal positrons, these equations are incorrect in principle. Even if in practice the inadequacy of the simple trapping model has not been evidentiated in many experiments on samples with a trap distribution probably very far from uniform, we believe that this is due only to the problems encountered in the analysis of the lifetime spectra in the short-time region. The continuing progress of the techniques used for measuring and analyzing positron lifetime spectra indicates that the moment has come for concentrating our attention also on effects once classified as of minor importance. Thus, in this talk the following points will be discussed: a) how can the effect of the disuniformity of the trap distribution become manifest; b) what are the accuracy limits required in an experimental observation of such an effect; c) once an effect has been observed, how can it be correlated to the morphology of the defect structure of the material.

The discussion will be reinforced with a practical example, taken from a recent study made by the Milano group in collaboration with the Centro Ricerche Fiat on annihilation in aluminum crystals plastically deformed at room temperature by uniform uniaxial compression. The experiment shows that the deviation from the simple trapping model is unmistakable for deformations over 12%, but probably already starts at a few % of deformation. These results can be correlated with the formation of a cell structure in the dislocation network, which is clearly shown by electron micrographies taken on the samples after the lifetime experiment. The analysis of the data, based on rate equations that take into account of the local variation of the trap density, leads to an estimate of the volume fraction occupied by the cell walls in good quantitative agreement with the estimates made on the electron micrographies.

VACANCY ANNEALING IN PURE AND CARBON-DOPED IRON

P. Hautojärvi

Laboratory of Physics, Helsinki University of Technology,
SF-02150 ESPOO 15, Finland

This paper gives a summary on positron studies of vacancies in pure and carbon-doped (50 and 750 ppm) iron [1-4]. Vacancies are produced by low temperature electron and neutron irradiations. Their annealing properties above 77 K are investigated by positron lifetime technique, which is sensitive to separate vacancy clusters from monovacancies. The analysis of the lifetime spectra is discussed and the results are presented in terms of concentrations of different vacancy-type defects.

The lifetime of free positrons in iron is 110 psec and that of trapped positrons in monovacancies is 175 psec. In all electron-irradiated specimens a distinct long lifetime of about 250-300 psec appears at stage III around 220 K showing clustering of mobile monovacancies. In doped iron the vacancy clustering is strongly reduced as the migrating vacancies are captured by carbon impurities. Asymmetric carbon-vacancy pairs are formed and the lifetime of trapped positrons at them is about 160 psec. At 350 K free carbon atoms get mobile and react both with vacancy clusters and with vacancy-impurity pairs causing a marked decrease in positron trapping. The carbon-vacancy pairs left above 350 K dissociate around 490 K resulting in another release of free vacancies in the lattice. During the heat treatments the trapped positron lifetime at vacancy clusters does not exceed 350 psec. Vacancy clusters anneal out between 500 K and 600 K.

In neutron-irradiated specimens the vacancy clustering is shifted down to 180 K and the clustering tendency is not affected by carbon atoms. This is explained by the correlated migration of vacancies within the collision cascades of fast neutrons, where the local vacancy concentration is high and much larger than the carbon concentration. The total positron trapping rate does not decrease during the correlated vacancy migration indicating that a major fraction of vacancies form agglomerates. The free migration of carbon atoms at 350 K leads to a marked decrease in the intensity of the longest positron lifetime due to carbon decoration of the vacancy clusters.

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A COMPARATIVE STUDY OF THE DENSITY OF ELECTRONS IN MOMENTUM SPACE FOR THE PERFECT LATTICE, THE VACANCY, AND THE LIQUID STATE OF Ni AS MEASURED BY POSITRON ANNIHILATION[*]

M. J. Fluss, L. C. Smedskjaer, B. Chakraborty, and M. K. Chason
Materials Science Division, Argonne National Laboratory,
Argonne, Illinois 60439, U.S.A.

Analyses of the Doppler-broadening energy spectra for positrons annihilating in solid Ni, and in liquid Ni (both above and below the melting point), will be reported. Comparisons will be made among the momentum distributions of positron-electron pairs annihilating in the essentially defect-free lattice, the vacancy, and the liquid state of Ni. An interesting similarity in the distribution of momenta is reported for positrons annihilating in vacancies at high temperatures and those annihilating in liquid Ni.

Ni samples (nominal purity 99.995 wt.%) were ion implanted with ^{58}Co and melted in-situ under ultra-high vacuum conditions in Al_2O_3 crucibles. The observed Doppler-broadening spectra for positrons annihilating in the essentially defect-free Ni, in thermally generated vacancies and in the liquid could all be described in terms of the sum of a parabolic and a Gaussian component, where the Gaussian (with standard deviation σ) corresponds to the broad momentum distribution of the more localized electrons. A rigorous theoretical estimate of variations in the σ of this Gaussian caused by electron and positron redistributions has not been attempted. Instead, the effect on σ due to changes in electronic structure has been studied assuming the positron to be in a zero-momentum plane-wave state. It has been shown that the major part of the changes in σ as a function of temperature could be explained on the basis of density alone, as could the solid liquid transition. Surprisingly, the present work also shows a clear similarity in the measured σ for vacancy-trapped positrons and positrons annihilating in the liquid Ni.

DEFECT SPECTROSCOPY WITH POSITRONS: CALCULATIONS

R. M. Nieminen

Department of Physics, University of Jyväskylä,
40720 Jyväskylä, Finland

and

M. J. Puska

Laboratory of Physics, Helsinki University of
Technology, 02150 Espoo, Finland

A versatile program for calculating localized positron states and their annihilation characteristics has been developed. The positron wave function is solved using finite element techniques in the true three-dimensional geometry for an arbitrary defect (vacancy, vacancy cluster, vacancy-solute complex etc.) The positron potential is constructed using the full electrostatic potential and the local-density approximation for the correlation potential. Lattice atom relaxations in and around the defect (including those induced by the positron) are incorporated. Lifetimes and momentum distributions of annihilation radiation are calculated for trapped positrons, with approximate but adequate inclusion of enhancement effects.

A number of applications to specific problems in positron defect spectroscopy will be discussed. These include (i) vacancy clusters in Al, V, Fe, Ni, Nb and Mo, (ii) vacancy-hydrogen and vacancy-helium complexes in Al; (iii) vacancy-carbon complexes in Fe. Special attention will be given to finding out how well positron studies can differentiate between defect complexes of different size and structure.

Experiences with the scheme have so far been very encouraging, and the predictive power of the method is deemed quite satisfactory. Efforts to extend the program to more involved situations are under way; these include defects in compounds with complicated crystal structures, defects at surfaces, and amorphous structures.

INVESTIGATION OF ELECTRON RADIATION DAMAGE IN
V, Nb, Ta, AND W BY POSITRON LIFETIME MEASUREMENTS

M. Haaf, W. Frank and H.-E. Schaefer

Institut für Theoretische und Angewandte Physik der Universität Stuttgart und In-
stitut für Physik, Max-Planck-Institut für Metallforschung, 7000 Stuttgart 80,
W-Germany

Crystal defects in group V and group VI bcc-refractory metals after electron irradiation (irradiation conditions see table 1) were investigated by simultaneous positron lifetime and Doppler broadening measurements. The lifetime spectra were analyzed in terms of lifetime components using the computer program POSFIT EXTENDED.

The positron lifetimes τ_f or $\tau_{1V} = \tau_2$ in the free or vacancy-trapped positron states were measured in the well annealed or irradiated specimens, respectively (table 1).

For V and W the dependence of the annihilation parameters from the irradiation dose was studied. At high irradiation doses in W deviations from the simple trapping model are observed. With the help of simultaneous electrical resistivity measurements in W the vacancy concentration and the positron trapping rate σ_{1V} (300K) = (1.5 ± 0.8) 10^{14} s^{-1} were derived. From a comparison with high-temperature experiments on W the temperature dependence of σ_{1V} could be estimated.

After isochronal annealing steps (t_a = 15 min) in the temperature range 120K $\leq T_a \leq$ 1500K (p < 10^{-5}Pa) the annihilation parameters were measured at constant temperature. Initial defect concentrations below positron saturation trapping were used.

In Nb and Ta the time constant τ_2 of the second lifetime component, which is due to the annihilation of positrons trapped by vacancies, could be observed up to the annealing temperature T_a = 420K. Therefore we conclude that single vacancies are not mobile below this temperature which is in agreement with the minimum temperature T_{1V} (table 1) for vacancy migration derived from thermal equilibrium positron annihilation and self-diffusion experiments at high temperatures. The formation of vacancy agglomerates and vacancy-impurity complexes at higher annealing temperatures will be discussed. A systematic study of the influence of N- or O-doping on the annealing of radiation induced vacancies is performed at present.

	V	Nb	Ta	Mo	W
T_i [K]	150	150	150	200	300
E_i [MeV]	3	3	3	3	3,5
ϕ_i [e$^-$m$^-$]	3.10^{20}- 10^{23}	3,5.10^{22}	7.10^{22}	7,4.10^{22}	10^{21}-2.10^{23}
τ_f [ps]	130	127	125	125	125
τ_{1V} [ps]	190	195	195	(185)	190
T_{1V} [K]	430	480	380	655	685

Table 1: Irradiation conditions (temperature T_i, electron energy E_i, and electron dose ϕ_i); positron lifetimes τ_f and τ_{1V} and vacancy migration temperature T_{1V} (estimated from high temperature experiments).

A MODEL OF THE LONG LIFETIME OF
POSITRONS TRAPPED BY INTERSTITIAL CLUSTERS

W. Frank*, A. Seeger*, and M. Weller**
Max-Planck-Institut für Metallforschung, Stuttgart

*Institut für Physik, Heisenbergstrasse 1,
D-7000 Stuttgart 80, F.R.G.
**Institut für Werkstoffwissenschaften, Seestrasse 92,
D-7000 Stuttgart 1, F.R.G.

In the literature it has been reported repeatedly that during annealing of irradiated metals through recovery stage III a new positron-lifetime component emerges which is longer than that ascribed to the annihilation of positrons in monovacancies. From this observation it was concluded that the new component originates from positrons trapped in vacancy clusters which are formed as a result of the free migration of monovacancies in Stage III. In the particular case of electron-irradiated α-iron the present authors have shown that this interpretation is not tenable and that the long lifetime component $\tau_2 \approx 400$ ps appearing in Stage III must be due to positrons trapped by interstitial clusters which are formed by self-interstitial migration in this recovery stage. In the present paper a model of the interstitial clusters and of the positron sites on these clusters which is capable of accounting for such a long lifetime component will be proposed. Moreover, attention will be focused on experiments which confirm the model.

HIGH-TEMPERATURE POSITRON LIFETIME
MEASUREMENTS AND ANALYSIS IN Mo AND W

R. Ziegler, H. Groß and H.E. Schaefer

Institut für Theoretische und Angewandte Physik, Universität Stutt-
gart, Pfaffenwaldring 57, 7000 Stuttgart 80, W-Germany

Measurements of the mean positron lifetime between room tempera-
ture and the melting points yield values between 130 ps and 173 ps
for Mo and between 133 ps and 175 ps for W. In both metals a well
developed S-curve behaviour is observed similar to earlier Doppler
broadening measurements.

The temperature dependence of the parameters obtained from a
two-component analysis of the lifetime spectra (FWHM of the spectro-
meter resolution function 300 ps) will be reported together with
simultaneously performed Doppler broadening measurements. Values
for the vacancy formation enthalpies will be presented.

INVESTIGATIONS OF VACANCIES IN Ta IN THERMAL EQUILIBRIUM
BY MEANS OF POSITRON LIFETIME MEASUREMENTS

A.G. Balogh, R. Gugelmeier, and H.E. Schaefer
Institut für Theoretische und Angewandte Physik, Universität Stutt-
gart, and Institut für Physik, Max-Planck-Institut für Metallfor-
schung, Stuttgart, 7000 Stuttgart 80, W-Germany

The positron lifetime spectra and the Doppler broadening of the 2γ-annihilation line were investigated on Ta between room temperature and the melting point. The measurements were performed under UHV conditions at pressures $p < 10^{-6}$ Pa using a sealed-source specimen.

The mean lifetime increases from room temperature ($\bar{\tau} = 124$ ps) up to 3000 K by 40 ps. The mean lifetimes, the results of a two-component evaluation, and the W and S parameters of the Doppler broadening spectra are used to obtain information on vacancies in Ta in thermal equilibrium. In particular the question of thermal positron detrapping from vacancies will be discussed.

POSITRON ANNIHILATION IN THE PLASTIC ZONE AT A CRACK TIP

Jiang Jian, Xiong Liangyue and Lung Chi-wei
Institute of Metal Research, Academia Sinica, Shenyang and
Institute of Solid State Physics, Academia Sinica, Hefei.

Ji Gaokun, Liou Nianching and Wang Shuying
High Energy Physics Institute, Academia Sinica, Peijing.

When a cracked sample is loaded, there is always a plastic zone in the vicinity of the crack-tip. Since the strin of plastic deformation is heterogeneous in the plastic zone, the distribution of density of crystal defects in this area is not uniform, and this may induce an ununiformity of positron annihilation effects.

Central cracked and single edge cracked α-Ti test specimens were prepared from 5mm thick plates. These specimens were annealed at $750°C$ in vacuum (about 10^{-3} torr) for three hours, and then loaded up to different stress levels in a tensile testing machine.

Both parameters, positron lifetime (^{22}Na) and Doppler broadening (Ge(Li)) lineshape were measured at room temperature. The relative change of τ_i and S parameters to that of crack-free, unloaded but heat-treated specimen as a function of loading levels are given in Fig.1. The τ_i and S parameters does not change in an elastic loading level as they are loaded below 1600kg, and then increased abruptly afterwards due to the defects caused by larger loading.

For single edge cracked specimen, the relative changes of S as a function of distance from the crack tip along the crack direction are given in Fig.2. It can be seen that the S parameters decrease monotonically along the crack direction untill a value is reached which agrees with that of the reference specimen within experimental error. The boundary of a plastic zone may be defined by this value and a contour of plastic zone may be roughly described. The size of plastic zone estimated by the positron annihilation method seems to agree roughly with that obtained from calculation by conventional fracture mechanics method.
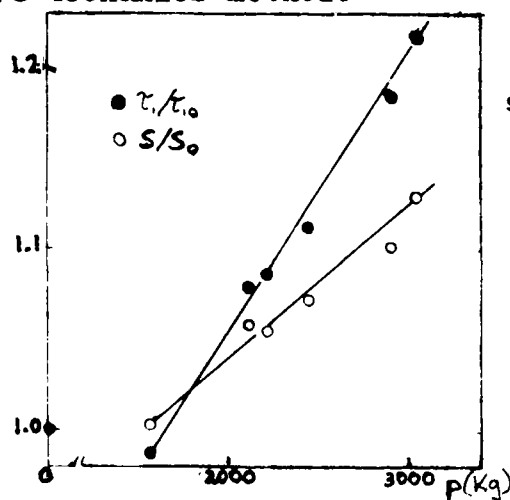
Fig.1 The relative changes of
τ and S parameter as a function of loading levels
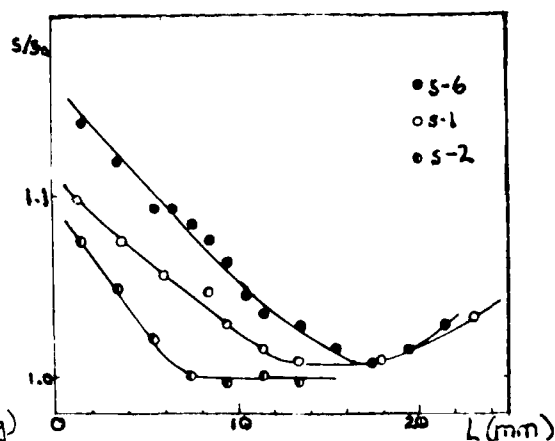
Fig.2 The relative changes of S
as a function of distance (for
single edge cracked specimen.)

COMPARISON BETWEEN THE STUDIES OF LATTICE DEFECTS
BY POSITRONS AND POSITIVE MUONS

Masao Doyama
Department of Metallurgy and Materials Science
Faculty of Engineering, The University of Tokyo
7-3-1 Hongo, Bunkyo-ku, Tokyo 113 Japan

It is well known that positron annihilation is quite sensitive to lattice defects. Positrons are trapped by vacancy type defects in many metals and alloys. Formation energies of a vacancy in many metals and alloys have been determined. by this method. Similar trapping of positive muons by vacancy type defects is expected, because positrons and muons are "isotopes". However, no trapping effect has been observed in positive muon experiments for vacancies at thermal equilibrium at high temperatures except some indication in indium. This may be due to the slow diffusion rate of positive muons and/or low binding energy between a positive muon and a vacancy.

The lifetime of muons is 2.2 microseconds which is much longer than that of positrons in metals. Therefore the spin relaxation or spin resonance of muons in transverse or longitudinal magnetic fields can be measured as a function of time after thermalization by detecting the positrons emitted in the muon decay. The wave function of a positive muon is more localized than that of a positron. The diffusion rate of positrons is much faster than that of muons. The gamma-gamma angular correlation emitted from positron annihilation gives the electron momentum when the positron is annihilated. However, the muon spin at the muon decay depends on the histeresis of the muon.

It has been shown that the quenched-in vacancies in pure aluminum trap positive muons at temperatures lower than 200 K. Applying the trapping model, the quantitative analysis of relative concentrations of vacancies and diffusion rate of positive muons in the matrix can be determined. From this experiment, the formation energy of a vacancy in pure aluminum was determined to be 0.68 eV, which is in good agreement with the value obtained by positron annihilation at thermal equilibrium.

The positive muon behavior in aluminum dilute alloys quenched from $600°C$ is also studied. At the temperatures below $10 K$, muons cannot reach impurity atoms whose fractional concentration is 5×10^{-4} within the lifetime ($2.2 \mu sec$). At about 15 K, almost all muons are trapped by impurity atoms of 5×10^{-4}. Muons are detrapped from impurity atoms at higher temperatures.

Positive muon behavior is quite sensitive to impurity atoms in metals. Positron behavior may be also sensitive to impurity atoms more than we think. The diffusion rate of positive muons can be measured from the depolarization behavior of positive muons. The positions of trapped positive muons can be estimated from the comparison of the calculated depolarization rate of positive muons. The lattice distortion around defects may be estimated. The corresponding behavior of positrons is more difficult.

Studies of point defects by positive muons and positrons are compared. Positive muon experiments can be also applied to one of the non-destructive testing techniques.

KINETICS OF AGGREGATION AND
ANNEALING OF DEFECTS IN HEAVILY
X-IRRADIATED ALKALI CHLORIDE
CRYSTALS STUDIED BY POSITRON ANNIHILATION

Stanley Stern and Werner Brandt
Radiation and Solid State Laboratory
New York University, New York, New York 10003, USA

During this past decade much understanding has been gained of the primary[1] and secondary[2] radiolytic processes in alkali halides and of the relationship[3] between the nature of damage and anneal. For example, Ausín and Alvarez Rivas[4] inferred from their thermoluminescence and optical-absorption experiments that annealing of F centers proceeds through interstitial-vacancy recombination. The kinetics is dictated by the distribution, depth, and kinds of interstitial-halogen traps created during radiolysis and formed during anneals. When thermally activated, F centers, moreover, may cluster into F_2, F_3, and F_4 centers.[5] A central shortcoming of integral techniques such as thermoluminescence, thermally-stimulated currents, ionic conductivity, or calorimetry for the study of such defective materials has always been the lack of definitive identifications of underlying microscopic mechanisms. Hence the mobile entity in F-center agglomerations is still not certain,[6,7] and the model [4] of the role of interstitials in the thermal bleaching of F centers, as observed by thermoluminescence, is controverted.[8]

We have undertaken positron-annihilation experiments with the homologous series NaCl, KCl, RbCl, CsCl to provide a new experimental basis to these kinetics studies. Isothermal and isochronal measurements of the coincidence count rate in a π-radian coincidence apparatus (PICA) give rates and activation energies for F-center aggregation and anneal.[9] The most significant trend in the positron data is that annealing proceeds faster the larger the cation, in agreement with the luminescence results of Ausín and Alvarez Rivas.[4] This trend supports the view that annealing is governed by vacancy-interstitial recombinations.

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POSITRON ANNIHILATION IN Pb^{2+} DOPED KCl SINGLE CRYSTALS

M. Chinnusamy, S. Ramasamy, T. Nagarajan and V. Manohar[+]
Department of Nuclear Physics, University of Madras,
A.C.College Campus, Madras 600 025, India.

The angular distribution of annihilation photons (ADAP) has been measured in pure KCl and in that doped with Pb^{2+} impurity to concentrations of 100 ppm, 550 ppm and 1050 ppm. After making the room temperature measurements, all the crystals were annealed at 650°C for 24 hours and then subjected to rapid cooling. The angular correlation measurements were carried out on these annealed crystals also. For the untreated samples, the intensity of the narrow components increases with the increase of impurity concentration. A comparision of the narrow components of the correlation curves of untreated and treated crystals, for a particular concentration, shows that there is no appreciable change in the intensity of the narrow component for 100 ppm impurity concentration, whereas for 550 ppm impurity concentration, the intensity of the narrow component of the heat treated sample is greater than that for the untreated sample and for 1050 ppm impurity concentration, the intensity of the narrow component for the heat treated sample, is less than that for the untreated sample. In untreated samples, as we increase the impurity concentration, the number of positive ion vacancies also increases and the annihilation of positrons trapped at positive ion vacancies (A centre annihilation) also increases, giving rise to an increase in the intensity of the lower momenta annihilation photons[1]. In annealed samples of 550 ppm, it seems that there is dissolution of impurities, i.e. major part of the associated vacancy-impurity pairs dissociate[2]. The host matrix expands as a result of the cumulative effect of the individual expansion around Pb^{2+} ions and of the relaxation of the cationic vacancies. Hence there is a decrease of electron density in the cationic vacancies giving rise to a decrease in the annihilation rate and photons of lower momenta. If the concentration of the divalent ions is too high such as 1050 ppm impurity concentration, it may not be possible to quench the crystal rapidly without some precipitation of impurities[3]. This subjects the host matrix to a compression, leading to an increase of electron density in the cationic vacancies. The decrease in narrow component intensity, in the heat treated crystal with 1050 ppm impurity is explained as due to the precipitation of impurities and compression of the host matrix.

[+]Present Address: Foster Radiation Laboratory, McGill University,
3610 University Street, Montreal P.Q.
Canada H3A 2B2

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ANNIHILATION OF A POSITRON IN A VACANCY IN GRAPHITE

M. Shimotomai, T. Takahashi, M. Doyama and T. Iwata*

Materials Science, Faculty of Engineering,
The University of Tokyo, Bunkyo-ku, Tokyo 113, Japan

* Division of Physics, Japan Atomic Energy Research Institute,
Tokai-mura, Ibaraki 319-11, Japan

The basic characteristics of positron annihilation in a
vacancy in graphite are measured by the combination of lifetime
and Doppler-broadening techniques and are compared with results
of calculation based on the LCAO-MO theory.

Highly-oriented pyrolytic graphite samples were irradiated
with 2 MeV electrons or with fission neutrons. Productions of
vacancies in the samples were confirmed by isochronal annealing
studies. The lifetimes of positrons in the perfect lattice and
in the vacancy are deduced to be 215±5 ps and 245±5 ps, respectively
by applying the trapping model. The Doppler-broadened lineshape
of the gamma-rays from the annihilating positron-electron pair
in the vacancy are measured in the directions perpendicular and
parallel to the basal plane of the graphite lattice.

The calculation of Doppler-broadened lineshape in the inde-
pendent approximation are made using the LCAO-MO wavefunctions
of the defect molecule (Coulson, 1963). A good agreement is
obtained between the experiment and the theory. The influence of
the charge state of the vacancy on the annihilation character-
istics is discussed.

DEFECTS IN AMORPHOUS SILICON FILMS

S. Dannefaer

Institute of Physics, University of Aarhus, DK-8000 Aarhus C, Denmark.

Positron lifetime measurements have been conducted in an attempt to investigate the properties of amorphous silicon films. The films were produced by: 1) evaporation, 2) sputtering using pure argon, and 3) sputtering using argon and fluorine. The thickness of the films varied between 7 and 11 μm and were deposited on single crystalline silicon. Using a 22-NaCl source, roughly 1% of the injected positrons annihilated within the film per 1 μm of thickness.

All three films gave rise to a new lifetime component, τ_2, having values in the range 400-500 ps. As many as 70% of the positrons annihilating inside the film were trapped by defects. During isochronal annealing, the τ_2 component disappeared around 700°C for the evaporated films, i.e. when crystallization of the film took place. For the sputtered films, however, the τ_2 lifetime persisted to 1300°C.

Another lifetime with a value of 2 ns was also observed in all three types of films. The intensity of this component (see Fig. 1) was 0,2% for both evaporated and argon sputtered films. The intensity for the sputtered film using both argon and fluorine was higher and increased in particular at 1050°C to 3%, i.e. ten times as much as for the other films.

It will be argued that vacancy clusters are responsible for the 400-500 ps lifetime component. The concentration of the clusters is estimated to about 60 ppm. In evaporated films these clusters disappear upon crystallization at 700°C, while in the sputtered films, argon seems to stabilize the clusters to much higher temperatures (~ 1300°C).

The effect of adding fluorine to the sputtered film will be argued to facilitate the formation of positronium in the vacancy clusters by saturating broken silicon bonds. The remarkable increase of I_3 at 1050°C is suggested to be a result of increased Ps formation probability due to the removal of argon trapped inside the clusters.
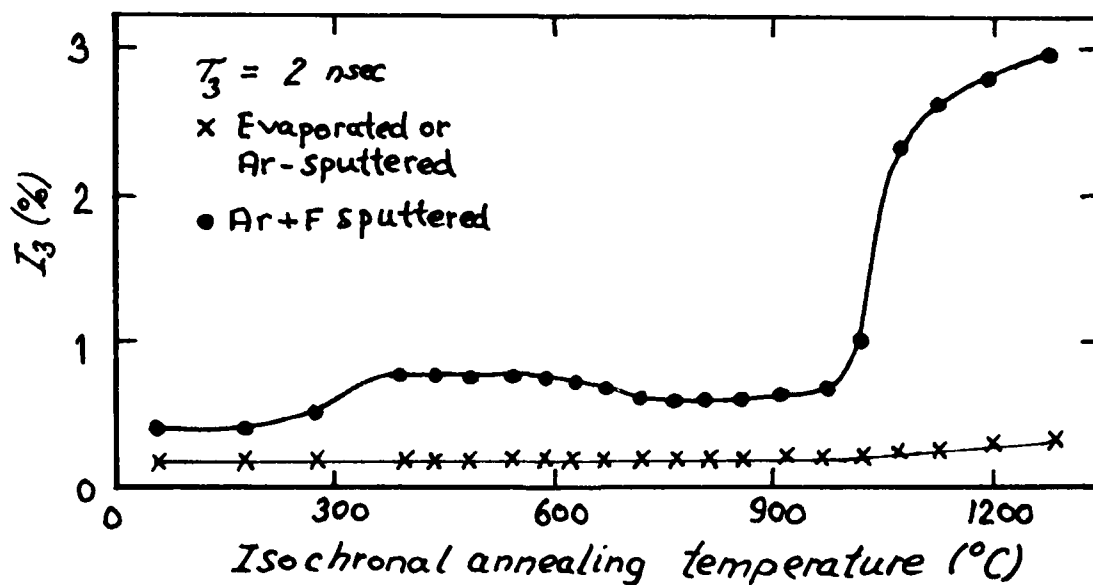
POSITRON MOBILITY IN GERMANIUM

T. McMullen
Department of Physics
Memorial University of Newfoundland
St. John's, NFld. Canada
A1B 3X7

The naturally occurring charge carries in the semiconductors diamond, silicon, and germanium are electrons and holes. An implanted thermalized positron also behaves as a charge carrier, and measurements of the mobility of this alternative charge carrier in semiconductors have now been made over a wide temperature range, including temperatures higher than those accessible by electron and hole mobility measurements. Mills and Pfeffer[1] found the positron mobility μ in Ge at 36K and 94K from drift velocity measurements. More recently, Jorch et al[2] have used a slow positron beam technique to determine the positron diffusion constant D (related to μ by the Einstein relation $D = \mu k_B T/e$) over the temperature range 300–1000K.

A theoretical expression for the positron mobility is compared with these experimental data. A deformation potential model is used for positron-acoustic phonon and positron-optic phonon scattering. Both scattering mechanisms are treated in a relaxation time approximation. The comparison yields estimates of the acoustic (E_1) and optic ($E_1{}^{opt}$) deformation potentials for positrons in Ge, and demonstrates that data in the 100–300K temperature region (which is not yet available) is needed to reduce the large uncertainties in these estimates. The possibility of observing positron scattering from thermally generated conduction electrons and valence band holes is investigated, but this scattering mechanism appears unlikely to be important at T < 1000K.

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TEMPERATURE DEPENDENCE OF THE TIME
AND MOMENTUM SPECTRA IN GERMANIUM

P. J. Schultz and I. K. MacKenzie
Department of Physics, University of Guelph
Guelph, Ontario, Canada
N1G 2W1

Recent measurements by H. Jorch et al, using the slow-β^+ beam at Brookhaven, suggested a thermally activated trapping mechanism which inhibited positron diffusion in single-crystal Ge. Supporting evidence has now been obtained from both Doppler broadening and lifetime measurements but, in both cases, the temperature dependence was so weak that it required the use of dual digital stabilization and unusual statistical precision in both types of spectrometry.

THREE - QUANTUM ANNIHILATION IN POWDERED ALUMINA.

C. Dauwe *,**   and Motoko Kwete *.

* ; Universite Nationale du Zaire, Campus de Kinshasa, B.P. 190
    Kinshasa XI, Republique du Zaire.
** ; Laboratorium voor Magnetisme, Rijksuniversiteit Gent,
    Proeftuinstraat 86, B-9000 Gent , Belgium.

The three - quantum annihilation method offers a convenient technique
for all cases where ortho-positronium is involved, specially in mat-
erials with high specific surface such as fine powders,gels,molecular
sieves etc..(1).We have measured the three-quantum yield in alumina,
Al2O3 of polishing grade and of three different particle sizes i.e
1 micrometer mean particle diameter (Specimen A),0.3 micron (Specimen
B), and 0.05 micron (Specimen C).For the greatest particle (A) the
three quantum yield P is some three times the Aluminium calibration
value of 1/372 ;this parameter P rises to a huge effect in smallest
particles (C) where it is some 25 times the Aluminium value.
Considering with Brandt(2) that ortho-positronium O-Ps is only formed
on the surface of the particles, and that the trapping of the therma-
lised positrons into these surfaces is diffusion limited, the three-
quantum yield can be written as ;

$$ P = (1/372 - \beta)(1 - \Lambda /R)^3 + \beta \qquad (a) $$

where $\beta = \dfrac{3\,\tau_3}{4\,\tau_0}$, τ_0 is the natural decay mean life of O-Ps in vacuum,

τ_3 is the total combined mean life of the O-Ps as can eventually been
measured in a two-quantum lifetime experiment, R is the particle ra-
dius for supposedly spherical particles, and $\Lambda = \sqrt{2 D \tau_B}$ where D is the

positron diffusion constant, and τ_B is the mean bulk lifetime of free
positrons.
It has been possible to adapt a relation(a) to our experimental data
giving the best values β = 0.0617 and Λ = 3.44 10^{-6} cm.
The value obtained for β thus predicts the existence of a long life-
time component τ_3 = 11.4 ns in these powders. We intend to search for
this component using a 4-detector O-Ps lifetime spectrometer which is
currently under construction.Knowledge of the mean bulk lifetime τ_B
will allow the accurate knowledge of the positron diffusion constant.

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ENHANCEMENT EFFECT ON POSITRON ANNIHILATION IN SOLID ARGON AND XENON

B.K. Sharma and Hanuman Singh

Department of Physics, University of Rajasthan, Jaipur-302 004,
INDIA

The life-time of a positron and the angular distribution of
the resulting annihilation photons have been computed for solid
argon and xenon using Chiba, Durr and Brandt formalism (1). In
contrast to the earlier results obtained on Salvadori and Carbotte
theory (2,3), the present calculation shows, both for Ar as well as
Xe, narrowing of the angular distribution curve when the effects
of electron-positron enhancement are included in the IPM results.

Interestingly, for both Ar and Xe, the angular distributions
computed from incoherent and coherent enhancement formulae look
identical, but the total areas of the distribution curves come out
to be different by a factor of about two in each case. The values
of the mean-life for positron thus computed, agree with the experi-
ment only for the coherent case.

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TWO-DIMENSIONAL ANGULAR CORRELATION; THEORY AND EXPERIMENT

R.M. Singru
Department of Physics, Indian Institute of Technology,
Kanpur, 208 016, India.

Recently different machines have been developed to experimentally study two-dimensional angular correlation of positron annihilation radiation (2D-ACPAR) curves

$$N_{\hat{n}}(p_y, p_z) = \int_{-\infty}^{+\infty} \rho_{\hat{n}}(\vec{p}) \, dp_x$$

where $\rho_{\hat{n}}(\vec{p})$ is the two-photon momentum density (TPMD) along the crystal orientation $\hat{n} = \{p_x, p_y, p_z\}$. Measurement of the 2D-ACPAR has provided us with a new method to test the electronic wave functions in metals and alloys by determining the TPMD which, in turn, depends sensitively on their band structure and Fermi surface. Theoretical calculations reported for Al, Cu, Cu-based alloys, V, VD_x, V_3Si etc. have demonstrated that the independent particle model calculations of the TPMD, $\rho_{\hat{n}}(\vec{p})$, performed by using standard band structure methods like OPW, APW, Hubbard's approximation scheme etc. provide a firm basis to compare the experiment with theory. Different steps involved in these calculations will be outlined and the effects of band structure on the 2D-ACPAR curves will be illustrated by showing specific results for Al, Cu and V. Role of the symmetry of electron wave function, many-body effects, relative enhancement of conduction and core electrons etc. will be discussed. In particular the importance of these effects for transition metals will be emphasized. The utility of the 2D-ACPAR method for non-dilute alloys will also be discussed with the help of examples of Cu-based alloys and VD_x.

Comparison of the experimental 2D-ACPAR data with theory is an important problem. One approach is to use the theoretical results for the TPMD, $\rho_{\hat{n}}(\vec{p})$, to predict the experimental 2D-ACPAR curves $N_{\hat{n}}(p_y, p_z)$ by taking into account the effects of detector resolution function, many-body enhancement, relative weightage of core and conduction electrons.[2] In another approach one uses the experimental results of the 2D-ACPAR surfaces, $N(p_y, p_z)$, for different orientations for reconstructing the momentum distribution. Such reconstruction can be carried out either to obtain a full 3D-momentum distribution or to obtain a function $\rho(\vec{k})$ reduced to the first Brillouin zone by Lock-Crisp-West theorem. These different methods to compare experiment with theory will be examined.

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PROGRESS IN THE DETECTION OF ANGULAR CORRELATION OF POSITRON ANNIHILATION USING HIGH DENSITY PROPORTIONAL CHAMBERS

A.A. Manuel, R. Sachot, P. Descouts and L. Oberli
Université de Genève, Département de Physique de la Matière Condensée
32, Boulevard d'Yvoy, 1211 Geneva 4, Switzerland

The study of electron momentum density using positron annihilation is often restricted by the small size of the Brillouin zone of the systems studied. Even with simple metals it can be very crucial to have a high angular resolution : k_F is about 4.3 mrad for Li. For the metallic compounds the trend is the same and we can encounter even smaller Brillouin zones. The consequence is that we need experimental set up with an high angular resolution, specially for the compounds where positron annihilation is one of the few methods that is useful actually to study electron momentum densities.

Another very drastic criteria in this field is derived from the structures we are interested in. They are correlated to the Fermi Surface, which is generally characterized by its complicated topology. For these applications, it has already been demonstrated that 2 D angular correlation techniques increases the power of the positron annihilation method.

We outline these two statements with some results obtained with an improved version of the high density proportional chamber system (1). The detailed description of this new apparatus is presented elsewhere during this conference, its main feature is an angular resolution of $(0.25 * 0.3)\text{mrad}^2$ for a typical counting rate of 100 cps.

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ELECTRON AND POSITRON STATES IN DISORDERED ALLOYS*

A. Bansil
Physics Department
Northeastern University, Boston, Mass. 02115, USA

Recent work concerning the nature of electron and positron states in disordered alloys is reviewed, with an emphasis on aspects most relevant for understanding the Compton scattering and positron annihilation experiments. In connection with the electronic problem, the essential elements of what may be viewed as a band theory of random alloys have emerged clearly during the last few years. This theory is based on the application of the average t-matrix (ATA) and the coherent-potential (CPA) approximations to the realistic muffin-tin Hamiltonian of the alloy. Within this framework, a variety of different properties of the one-electron equilibrium structure (e.g., complex energy bands, Fermi surface, average density of states, electron momentum density) have been investigated. The extensions of the theory to discuss magnetic phenomenon, band spectroscopies of alloys, etc., are at various stages of development. Illustrative examples of transitions and noble metal alloys will be presented.

As a step towards understanding the nature of positron states, we discuss the properties of a single thermalized positron placed in an alloy of (repulsive) muffin-tin potentials, assuming that there are no electrons. This hypothetical problem is amenable to treatment by the aforementioned ATA and CPA techniques, and its study permits a considerable insight into the characteristic effects of disorder on the e^+-states. It should be emphasized that disorder influences the positron in a way which differs qualitatively from the case of an electron. The positron is repelled by the ions and tends to sample the outer parts of the Wigner-Seitz cell, whereas the electrons are attracted towards the ionic cores. Also, the positron would sit at the bottom of the associated conduction band (at T=0 K). By contrast, the most important electronic states in the metal lie in the vicinity of the Fermi energy, well above the lowest occupied electronic energy level. Recent results on Cu-based solid solutions will be used to compare ATA and CPA in the positron problem, and to delineate physically important effects, such as, the disorder vs. thermal smearing of the e^+-states.

The question of incorporating the influence the positron spatial distribution on the angular correlation of annihilation radiation (ACAR) from alloys has begun to be investigated only very recently. The simplest approach, in the spirit of the independent particle model, is to replace the average of the product of the positron and electron Green's functions, i.e., the quantity $<G_+G_->$ (which enters the consideration of ACAR), by a product of the averages, i.e., by $<G_+><G_->$. However, the effects of the "vertex" corrections so neglected need to be explored, since these corrections physically represent the preferential "affinity" of the positron towards one of the constituents. These and related issues will be discussed.

SPIN DEPENDENT 2D ACAR MEASUREMENTS IN GADOLINIUM*

K. R. Hoffmann and S. Berko
Physics Department, Brandeis University
Waltham, Massachusetts 02254, U.S.A.

The spin dependent momentum density of Gd was studied by two dimensional angular correlation of annihilation radiation (ACAR) measurements,[1] using the spin polarized positron technique.[2] The ferromagnetic electrons of Gd were spin aligned parallel and antiparallel to the positron spin using a saturating 22 kG magnetic field at ~100 K. The momentum resolution of the apparatus was 0.6 and 1.7 mcx10^{-3} along the p_z and p_y directions. Experiments were performed with the integration direction p_x along (0001) and (11$\overline{2}$0). Using the filtered back-projection technique we have reconstructed the three dimensional momentum density for a few planes perpendicular to the (0001) direction. To obtain the reduced scheme Fermi surface (FS) topology we use the two and three dimensional extension of the LCW theorem,[3] by convoluting the distributions with the projections of the reciprocal lattice. The shape of the reconstructed effective long-slit data from the 2D ACAR results fits well the early 1D data.[4,5] The anisotropies observed will be discussed in terms of the topology of the majority and minority spin Fermi surfaces[6] of Gd.

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STUDIES OF THE FERMI SURFACE OF
TANTALUM BY 2D ACAR MEASUREMENTS*

F. Sinclair, K. R. Hoffmann, and S. Berko
Physics Department, Brandeis University
Waltham, Massachusetts 02254, U.S.A.

Using a 64-detector apparatus[1] we have made two dimensional angular correlation of annihilation radiation (2D ACAR) measurements on a single crystal of Tantalum. If $\rho(\underline{p})$ is the momentum distribution of the annihilating positron-electron pair, our apparatus measures $N(p_y, p_z) = \int \rho(\underline{p}) dp_x$ with a resolution of .6 mrad in p_z and 1.7 mrad along p_y. Full 2D ACAR measurements have been made using the same single crystal in two different orientations: p_z, p_x were chosen along [110], [$\bar{1}$10] and then [110], [001].

We have convoluted our data with a projection of the reciprocal lattice and compared the result with predictions based on the APW Fermi Surface (FS) calculation of Mattheiss.[2] A three-dimensional computer model of algebraically simple surfaces was least-squares fit to the calcuated FS modified by the results of de Haas-van Alphen measurements.[3] This enables us to model the effects of our resolution and produce a good fit to the data, especially in [001] integration direction.

We have also made measurements on a single crystal of Ta with 12% Hydrogen in the [110],[$\bar{1}$10] orientation. The main difference from the pure metal when the data is folded into one Brillouin Zone is a diminution of the amplitude of the structure. Integrating our data along the appropriate directions leads to very good agreement with the earlier long slit data of Hasegawa,[4] but in two dimensions it is clear that the changes produced by the introduction of Hydrogen cannot be ascribed simply to changes in the FS at the N-points.

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THE AUTOCORRELATION FUNCTION $B^{+-}(r)$ IN POSITRON ANNIHILATION PHYSICS*

S. Berko, W. S. Farmer, and F. Sinclair
Physics Department, Brandeis University
Waltham, Massachusetts 02254, U.S.A.

During the recent years the Fourier transform $B(r)$ of the electronic momentum space density $\rho(p)$ has been successfully used to interpret momentum density measurements by the Compton profile (CP) technique.[1] The function $B(r)$ represents the autocorrelation function (AC) of the electron wavefunctions in real space and is symmetrical to $F(p)$, the usual form factor appearing in diffraction theory (which measures the AC function of the momentum space wavefunction). Paralleling the definition of $B(r)$ we can define a positron-electron $B^{+-}(r)$ as the Fourier transform (FT) of $\rho^{2\gamma}(p)$ where $\rho^{2\gamma}(p)$ is the momentum density of the positron-electron system, projections of which are measured by the 2γ angular correlation experiments (1D and 2D ACAR).

A fundamental reconstruction theorem states that the FT of the 1D and 2D ACAR results yield $B^{+-}(0,0,z)$ and $B^{+-}(0,y,z)$. We shall present several examples of these B^{+-} functions both from 1D and 2D ACAR data. Because of the presence of the positron wavefunction $B^{+-}(r)$ cannot be related directly to $B(r)$, yet it carries interesting physical significance. In particular the use of $B^{2\gamma}(0,0,z)$ to measure the Fermi radius of simple metals will be analysed for Al, and compared to the CP data. Two dimensional $B^{2\gamma}(y,z)$ will be shown and discussed for several pure metals and for V_3Si. The use of B functions for reconstruction algorithms will be also discussed.

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TWO-DIMENSIONAL ANGULAR CORRELATION STUDIES
OF DEFECT AND DEFECT-RELATED PROBLEMS IN METALS

R. N. West
School of Mathematics and Physics,
University of East Anglia, Norwich, England.

The study of positron-defect trapping ρ   a during the last ten years
has brought about significant advances in bo   iment and theory clearly
exposing both the strengths and weaknesses o   sitron techniques in
studies of both equilibrium and nonequilibriu   nt defect problems. A major
problem in the interpretation of many results   is far has been the separation
of factors depending essentially on the concentration of defect traps from a
variety of other parameters that describe the trapped positron states. Here,
the development of two-dimensional angular correlation machines which provide
much more detailed momentum spectra than their more common 1-d counterparts
promises considerable advance. Two-dimensional momentum spectra, obtained on
the UEA machine,[1] and having relevance to a variety of different positron-defect
problems will be presented and the implications of their content discussed.

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TWO-DIMENSIONAL ELECTRON-POSITRON MOMENTUM DENSITIES IN THE HCP METALS Mg, Zn, AND Cd

P. A. Walters, J. Mayers and R.N. West
School of Mathematics and Physics
University of East Anglia, Norwich, England.

Two-dimensional angular distributions for two-different orientations of similarly cut single crystals of Mg, Zn, and Cd have been obtained on the UEA 2-d machine[1]. Unlike their earlier studied 1-d counterparts these distributions show clear anisotropies throughout their range reflecting both higher momentum components (HMC) in the particle wavefunctions and appreciable deviations of the Fermi surfaces from the simplest free electron spherical form. The HMC are consistent with existing theories in which the c-direction periodicity produces the dominant effects in both electron and positron wavefunctions. Within the range $p < p_F$ the observed anisotropies are well reproduced by electron pseudopotential theory.

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TWO-DIMENSIONAL ANGULAR CORRELATION OF POSITRON ANNIHILATION RADIATION FROM NEUTRON-IRRADIATED ALUMINIUM

R.N. West and P. Walters
University of East Anglia, Norwich, England
and
J.D. McGervey
Case Western Reserve University
Cleveland, Ohio 44106, U.S.A.

We have measured the two-dimensional angular correlation of positron annihilation radiation from single crystals of neutron irradiated aluminium containing facetted voids and other defects. For angles less than 10 mrad the 2-d angular distribution is essentially isotropic. This is contrary to the predictions of an independent particle calculation which assumes that the positrons are trapped in surface states on the void walls, which in these samples are primarily [111] planes. The implications of this disparity and other aspects of the results in respect to the nature of the positron states in voids will be discussed.

2D ANGULAR CORRELATION EXPERIMENTS ON αCuGe AND αCuZn ALLOYS: THE RECONSTRUCTION OF MOMENTUM DENSITIES FROM DATA

L.M. Pecora and A.C. Ehrlich

Code 6331, Naval Research Laboratory, Washington, DC 20375

Two dimensional-angular-correlation-of-gamma-ray experiments have been done on single crystals of $\alpha Cu_{1-x}Ge_x$ ($0 \leq x \leq 0.08$) and $\alpha Cu_{1-x}Zn_x$ ($0 \leq x \leq 0.25$). Data was taken using a unique set of collimators fabricated from die flat stock and Tantalum tubing. Each experiment yielded data in 6-7 directions in a plane in momentum space (usually (110) or (111)) from $0 \rightarrow \geq 12$ mrad. The data was analyzed by first deconvoluting using a statistical regularization scheme.[1] The deconvoluted data was then used to reconstruct the momentum density $\rho(\vec{p})$ of each alloy in the appropriate data plane of momentum space.[2] A study of the ability of this data analysis scheme to reproduce various details and the propagation of errors through the analysis showed that 6 directions suffice to represent $\rho(\vec{p})$ well in either (110) or (111) for these systems. In particular, analysis of a model $\rho(\vec{p})$ for the (110) plane of Cu shows that the reconstruction process does not worsen the resolution of the data. Comparison of the model results with Cu(110) results also allows the accurate determination of the true FWHM of the resolution in the final $\rho(\vec{p})$ calculation. Thus $\rho(\vec{p})$ is known reasonably well in the full data plane for all the alloys investigated. These results were used to plot $\rho(\vec{p})$ as both surface plots and contour plots in the entire data plane as well as to examine $\rho(\vec{p})$ along any direction in the plane. In addition, by scaling each $\rho(\vec{p})$ to the pure Cu momentum density the Fermi radius in various directions in the momentum plane were determined. Comparisons of $\rho(\vec{p})$ along certain directions with the model Cu (with varying Fermi radii) and with self-consistent APW results for Cu[3] also suggested other changes which might be taking place in $\rho(\vec{p})$ (and, hence, the wave function) in these alloys upon addition of the solute. Application of these techniques to the data from αCuGe alloys showed that at low concentration the Fermi surface in several directions does not grow as fast as rigid band results[3] and may even shrink in the [100] direction. This is in agreement with data by Suzuki, et al[4] and is also suggested in CPA calculations by Bansil, et al.[5] Another feature of $\rho(\vec{p})$ in the CuGe alloys was in the large change with Ge content in the anisotropy in $\rho(\vec{p})$ at 6-8 mrad between the [110] and [100] direction. In this region the conduction band does not contribute. In Cu the anisotropy is such that $\rho_{[110]} > \rho_{[100]}$ in these regions and was explained by Mijnarends[6] as resulting from s-d hybridization. The CuGe alloys show a reversal of this anisotropy systematically with increasing Ge concentration until for the largest Ge concentration $\rho_{[100]} > \rho_{[110]}$. The changes are too large to result from resolution effects and have been interpreted as changes in s-d hybridization.[7] Comparisons with the APW $\rho(\vec{p})$ calculations for Cu allows an estimation of the change of s, p, and d populations in αCuGe in these regions of momentum space. Similar analyses of αCuZn data show that at low concentrations the rate of growth of the Fermi surface is faster than the rigid band APW results in certain directions. The [110]/[100] anisotropy in the 6-8 mrad regions also changes, but the changes appear to agree with model resolution effects resulting from Fermi radius changes and hence, no s-d hybridization changes are postulated here.

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THE GENERATION AND DETECTION
OF MONOENERGETIC POSITRONS*

L. D. Hulett, J. M. Dale
Analytical Chemistry Division, Box X
Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830, U.S.A.
S. Pendyala
State University of New York, College at Fredonia
Fredonia, New York 14063, U.S.A.

In the past 3-4 years, large improvements have been made in techniques for generating monoenegetic positrons. The authors have reported (1) a procedure using tungsten moderators that has proven to be very practical. High intensities of positrons can be generated, even under adverse vacuum conditions. Thus the method is useful for experiments involving gases as well as solids. Since our initial report (1), efforts have been underway to optimize the tungsten moderator technique. Polycrystal, single crystal, and fine particle surfaces are under study. Also, certain alloy surfaces are being investigated. Positron yields for these new moderators will be reported.

The authors have recently demonstrated that the channel electron multiplier array (microchannel plate) can be used as a position sensitive detector in positron spectrometry. We have shown that the annihilation gamma rays do not cause high backgrounds. Efforts are underway to record LEPD patterns with this device. Progress will be reported.

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PRODUCTION OF SLOW POSITRON BEAMS WITH AN ELECTRON LINAC

R. H. Howell and R. A. Alvarez
Lawrence Livermore National Laboratory
Livermore, California 94550

Intense, pulsed slow-positron beams can be produced from the energetic electron beam of an electron LINAC. The mechanism of positron production-moderation has been investigated and some of the characteristics which result in optimum positron production have been identified. These characteristics include the energy of the electron beam, the thickness of the electron-positron converter, the preparation of the positron moderator and the quality of the tuning of the electron beam. The production efficiency has been measured for a series of positron converter-moderator geometries. The effect of changing the converter thickness has been studied and the best thickness identified. The effect of changing the energy of the electron beam has also been determined.

Using a tungsten moderator and the best set of characteristics determined thus far, the efficiency of producing slow positrons from LINAC electrons has been measured to be 1.5×10^{-6}. With this efficiency the beam available at the electron LINAC can produce slow positron beams with up to 0.5 namp average current in long pulses and 6×10^5 positrons in short pulses of 20 nsec duration and $1440 \ \text{sec}^{-1}$ repetition rate. These pulses may be bunched to shorter duration. Also the correlation between flight time and energy can be used to make the beam nearly monoenergetic, partially eliminating the need for brightness enhancement.

The present status of the efficiency measurements will be presented and the progress toward a permanent beam station for use of these beams by the positron community will be discussed.

POSITRON LIFETIME MEASUREMENTS WITH A
β+-γ-SPECTROMETER ON In, Pb and Pt

W. Weiler, H.E. Schaefer and K. Maier

Institut für Theoretische und Angewandte Physik der Universität Stuttgart und Institut für Physik, MPI für Metallforschung, 7000 Stuttgart, W-Germany

A β+-γ-spectrometer has been built up according to the suggestion of Maier and Myllylä /1/. By means of a magnetic sector field positrons in the energy range of 600 - 800 keV are selected from a 500 Ci ^{68}Ge source with a diameter of 6 mm. The start signal for the time measurement is produced by the positrons passing a 0.4 mm thick plastic scintillator. In order to measure exclusively stop signals from the specimen the two 511 keV-annihilation quanta are monitored in coincidence.

The resolution function of the spectrometer can be measured by using the prompt β−-γ-emission of ^{122}Sb with similar energies as in the case of the ^{68}Ge positron emitter. At the present time a FWHM-value of 360 ps is obtained with a coincidence count rate of 20 cps in the lifetime spectrum, and 5 x 10^3 cps in the start detector.

So far experiments between 77 K and 650 K can be performed and measurements on In, Pb and electron irradiated Pt will be discussed.

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APPLICATIONS OF THE POSITRON ANNIHILATION
DOPPLER TECHNIQUE IN NON-DESTRUCTIVE EVALUATION
OF MATERIALS[†]

C.F. Coleman, A.E. Hughes and F.A. Smith
Atomic Energy Research Establishment, Harwell,
Didcot, OX11 ORA, United Kingdom

There are now numerous examples of the application of positron annihilation techniques to materials problems, but still very few where an attempt has been made to examine non-destructively real engineering components or test pieces of complex geometry from materials testing programmes. Such a capability must be demonstrated if positron annihilation is to make a practical contribution to non-destructive evaluation. The Doppler technique offers the best hope in this respect, since it is not too restrictive from a geometrical point of view and can make measurements reasonably quickly. ^{68}Ge sources give greater penetration of positrons into the sample than ^{22}Na and require less rigorous control of surface preparation and contamination.

Measurements of the change in the Doppler peak shape parameter S at stages in the fatigue life of batches of cylindrical geometry test pieces of a titanium alloy (IMI 550) show that the largest changes occur prior to crack initiation and correspond to the detection of defects produced by plastic deformation processes. The stage in the fatigue life at which damage accumulates varies somewhat from sample to sample, and the damage itself is often distributed non-uniformly over the gauge length of a test piece. We have measured the spatial distribution of defects produced by non-uniform plastic deformation in a wide variety of sample geometries using small backed ^{68}Ge contact sources less than 1 mm in diameter. This method is particularly useful for providing quantitative information about the plastic zones near stress raisers such as holes, grooves, notches and cracks, and for detecting inhomogeneities in materials. Examples of the application of this technique to steel and titanium alloy samples of various shapes will be shown to demonstrate the extent to which the Doppler technique can be developed as a practical tool for evaluating mechanical damage in engineering alloys.

ANALYSIS OF SMALL VARIATIONS
OF POSITRON LIFETIME SPECTRA

G.Aldi[a], A.Dupasquier[a,b]

[a]Istituto di Fisica del Politecnico, Milano, Italy
[b]Gruppo Nazionale di Struttura della Materia del CNR,
Italy

Inaccuracies in the absolute analysis of multicomponent life-time spectra often limit the study of small perturbations of annihilation characteristics. We propose a new method of analysis, based on the direct comparison of the perturbed spectrum with a reference, leading to the determination of the difference spectrum. The main advantage of the method ensues from the cancellation of spectral components unaffected by the perturbation. In most cases full quantitative and qualitative characterization of an observed effect can be obtained from the difference spectrum without a deconvolution procedure. The first moment of the difference spectrum, which can be obtained with great accuracy without specified assumptions on the resolution function, is the mean lifetime difference, a physical parameter of well defined meaning. The identification of the perturbed annihilation characteristics (lifetimes and/or intensities of specific components, which does not come from the evaluation of the mean lifetime, can be obtained from simple shape parameters of the difference spectrum.

The choice of the shape parameters will be discussed on the basis of calculated curves, for the most frequently occurring cases: a) lifetime variation; b) intensity variation; c) combined lifetime/intensity variation as predicted by the trapping model.

Practical examples with measured spectra will also be given.

ANALYSIS AND INTERPRETATION OF
POSITRON LIFETIME SPECTRA

H. Groß, P. Schmid, A. Seeger and H.E. Schaefer

Institut für Theoretische und Angewandte Physik der Universität Stuttgart und Insti   für Physik am Max-Planck-Institut für Metallforschung, Stuttg..., 7000 Stuttgart, W-Germany

Using lifetime measurements on aluminum between room temperature and the melting point and numerical simulation experiments we have investigated problems of spectrum analysis and interpretation in metals.

When the simple trapping model is fitted to the temperature dependence of our mean lifetime results on Al the vacancy formation enthalpy $H_{1V}^F = (0.66 \pm 0.04)$ eV is obtained.

In the analysis of the lifetime spectra uncertainties arise in connection with the determination of the resolution function. Analogous problems are also observed in simulation studies. The value of the time zero parameter T_O of the lifetime spectrum as determined in the analysis is influenced by the quality of the resolution function and also depends on the model applied. This makes the discussion of the results difficult but there are indications that the simple trapping model is not a sufficient description of the experimental data on Al. Thus, from the temperature dependence of the numerically extracted lifetime parameters higher H_{1V}^F values are obtained than from the mean lifetimes. The results will be discussed in terms of generalizations of the simple trapping model.

ASSESSING AND MAXIMIZING THE INFORMATION CONTENT OF
LIFETIME SPECTRA FROM INFORMATION THEORY[a]

D. M. Schrader
Chemistry Department
Marquette University
Milwaukee, WI 53233 U.S.A.

It is usual to assume the annihilation photon count to be of the form

$$C(t) = \theta(t)\sum_{i=1}^{N}\alpha_i(\tau_i^{-1}e^{-t/\tau_i}) = \theta(t)\sum_{i=1}^{N}I_i e^{-t/\tau_i} \tag{1}$$

where $\theta(t)$ is the unit step function. The raw laboratory data (i.e., the MCA contents) consists of $C(t)$ convoluted with the instrumental resolution function and averaged over the width of each channel, with Poisson scatter and a constant background. The "lifetime spectrum" is a tabulation of N pairs of $\alpha - \tau$ values, usually obtained from the raw laboratory data by POSITRONFIT[1] or a successor.

Equation 1 can be generalized so that the right hand side is a Laplace transform of $I(k) = I(\tau^{-1})$. Then the data extraction problem is transformed from one of minimizing a sum of squared deviations to one of inverting a Laplace transform. A canonical solution of the inversion problem is achieved by appealing to an expansion of $I(k)$ in the basis set of the eigenfunctions of the transform[2]. This exercise reveals that (a) the information content per unit length of absicissa is constant in a plot of α vs. log k or log τ; (b) a resolution factor ρ can be calculated directly from the MCA contents, and two lifetimes $\tau_i<\tau_j$ can be resolved only if $\tau_j/\tau_i > \rho$; (c) the Shannon number of information theory can be calculated directly from the MCA contents, so that one can tell before the data extraction step, and during data collection, how many features of a plot of α vs. log τ can be resolved; and (d) the Shannon number can be expressed as an explicit function of controllable parameters. Our numerical experiments suggest that our current methods of data extraction do not provide all the information contained, and indicate how the information content can be substantially increaed.

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A SIMPLE POSITRON SPIN ANALYSER USING
A Ge DETECTOR*

T. Akahane and S. Berko
Physics Department, Brandeis University
Waltham, Massachusetts 02254, U.S.A.

We report on a convenient method for measuring the spin polarization of positrons with a Ge γ ray detector. Positron spin polarization and helicity is usually measured by Mott and Bhabba scattering, or by the Zeeman splitting of Positronium (Ps) through lifetime spectra[1], or angular correlation of annihilation radiation (ACAR) experiments.[2] The methods have intrinsically low efficiencies and/or require strong magnetic fields. The ACAR measurements in saturated ferromagnetic materials provide another polarization sensitive method,[3] but suffers from low efficiency because of the geometry of the usual ACAR setup. We report the first measurement of the spin dependent momentum density by positron annihilation from saturated ferromagnets using an intrinsic Ge detector.

Doppler broadening measurements were carried out on a sample of Hyperco – a magnetically soft iron alloy, designed to close the magnetic circuit of a small C-shaped electromagnet. The test positrons were collimated from a 2 mCi ^{68}Ge source and made to strike the saturated specimen at an incident angle of 60° to the spin aligned electrons. A collinear NaI(Tl) detector was used in coincidence with the Ge detector to reduce the background. Magnetization was reversed every 9 minutes. The results are similar to the early ACAR measurements in Fe by Berko and Zuckerman,[4] but the Ge detector geometry provides a large increase in efficiency. In order to use the technique as a spin polarimeter, it is sufficient to measure the parameter $P \equiv \int_{E_1}^{E_2} [(N_\uparrow(E) - N_\downarrow(E)] dE / \int_{E_1}^{E_2} [(N_\uparrow(E) + N_\downarrow(E)] dE$, where $\uparrow$ and $\downarrow$ represent the field parallel and antiparallel with the original positron momentum and E_1 and E_2 was selected for optimizing the magnitude and the precision of P. For the range of 2.3 keV to 5.1 keV from the centroid of N(E) (corresponding to 9 mrad to 20 mrad in ACAR) we obtained P=(2.0⁺⁻.1)%. As a test we changed the incident e⁺ beam angle to 30° and obtained F ₁.1±0.1)%. We checked spurious effects by placing a 0.35 mm thick Cu foil over the iron-alloy specimen, and obtained P≈(0.08±0.1)%.

The advantages of this spin analyzer method are as follows: a) the technique does not require a large magnet, and thus can be combined easily with other experiments such as slow positron beams in UHV. b) Counting efficiency is relatively high. c) Longitudinal as well as transversal spin polarization can be measured. On the other hand, it is difficult to obtain an absolute value of the spin polarization, since that would require a good knowledge of the spin depolarization in the sample.

The technique is also well suited to study the spin dependence of the high momentum component of the electron wavefunctions in ferromagnets.

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ON POSITRON STUDIES OF MOLECULAR CRYSTALS

Morten Eldrup
Chemistry Department, Risø National Laboratory,
DK-4000 Roskilde, Denmark

Molecular crystals have been the subject of many positron annihilation investigations. Some of these studies have recently been briefly reviewed[1-4]. The present talk will sketch the experimentally available information about positron and positronium states in molecular crystals, pointing out problems in our understanding. The talk will mainly deal with some recent studies, concentrated around the defect properties of the crystals.

Positronium (Ps) is formed in many molecular crystals and the measurements have mainly aimed at obtaining information about the Ps formation and behaviour and through this - if possible - about the solid under study. Ice, which has been investigated in considerable detail, seems to provide a relatively simple picture of Ps behaviour in molecular crystals. Very narrow ($\gtrsim$ 1 mrad) para-Ps central and side peaks in angular correlation curves at low temperatures give evidence of delocalized, thermalized Ps. Three lifetime components can be associated with "free" positrons, para-, and ortho-Ps, and within experimental uncertainty the ratio between the observed para- and ortho-Ps yields are 1/3. On heating, doping, or irradiation Ps is seen to localize (i.e. get trapped) at the defects introduced. In other molecular crystals the picture is less simple. For example, there is no evidence of delocalized Ps in the angular correlation curves, in some cases even no narrow components which may be associated with para-Ps in spite of the presence of long-lived components in the lifetime spectra attributable to ortho-Ps. Such deviations from a simple picture will be discussed. Defects introduced either by doping with impurities or by heating in both plastic and ordinary ("non-plastic" or "brittle") crystals have been the subject of a number of recent investigations. Some of these will be summarized, illustrating e.g. the derivation of vacancy formation energies and of a relationship between ortho-Ps lifetimes and vacancy volumes. A conclusion may be that in spite of the shortcomings in our detailed understanding of the Ps states in molecular crystals the positron annihilation techniques are able to give new information about defects, especially of vacancy type, in such crystals.

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MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS-1963-A

POSITRONIUM FORMATION IN CONDENSED
MATTER AND HIGH-DENSITY GASES
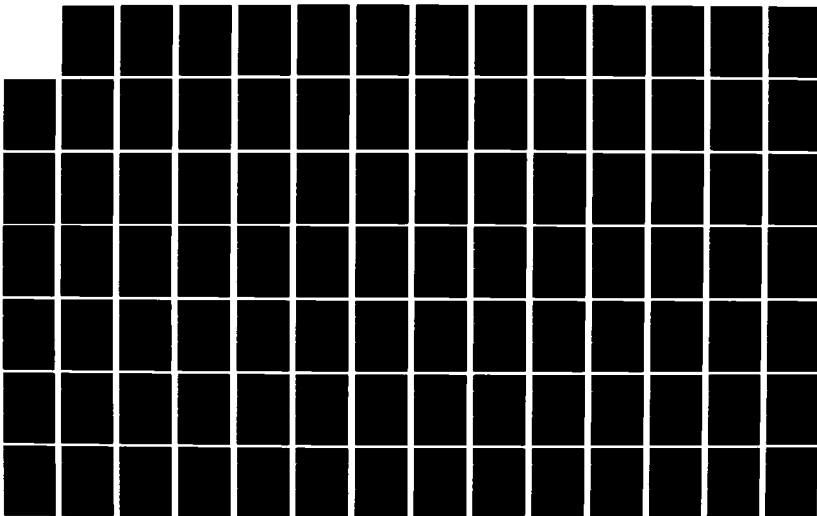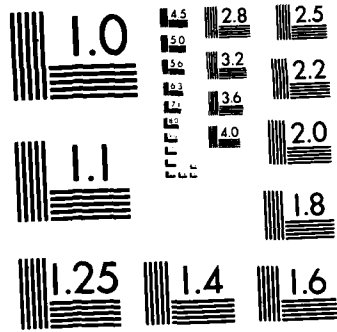
O.E. Mogensen

Chemistry Department, Risø National Laboratory,

DK-4000 Roskilde, Denmark.

The present talk is intended to be a fairly elementary review of recent positronium (Ps) formation research. In particular the correlation between Ps yield work and radiation chemistry studies will be emphasized. The detailed content of the talk will depend somewhat on whether it is to be presented early or late at the conference.

Concerning the science sociology aspects of Ps formation the following can be said. Until 1973 the Ore model was the only used model in Ps formation research. However, it was soon realized that the Ore model cannot explain the measured apparent Ps yields (e.g. in CCl_4, C_6H_5I, etc.). Hence, hot Ps reactions was included in the interpretations. Furthermore, the effects of "free volume" in condensed matter have been used by W. Brandt et al. to explain the measured apparent Ps yields. It must be realized that it is very difficult to disprove the validity of the three combined models as many of the processes used in the models have not been studied yet. The fourth model for the explanation of the apparent measured Ps yields - the spur model - was proposed by me in 1973. Today the spur model is roughly speaking accepted although some scientists still prefer the use of the older models. The science-sociological developements between 1973 and 1981 can be characterized as the first part of a change in "paradigm" in the T. Kuhn sense. Today the spur model is strongly debated in muonium formation research.

In the spur model Ps is formed by a reaction of the positron with one of the excess electrons created as a result of the slowing down of the positron in the last part of its track the socalled positron spur. It is a two-step process. First, the spur is created (ionizations, etc.) and the positron and the secondary excess electrons are slowed down to (or near to) thermal energies. Secondly, the spur specie including the positron and the excess electrons react with each other or escape from the spur. Hence, the Ps formation process must compete with other spur processes during the spur "collapse". Spur and track processes are studied mainly by radiation chemists.

The spur model of Ps formation is accepted mainly because the model can explain the experimental results in most cases, and also because many results have been predicted by use of this model. For instance the Ps yield is much lower in cyclohexane and decalin than in other hydrocarbons because the positive hole is much faster in those two liquids. Correspondingly if the fast hole is trapped on a massive molecule the Ps yield increases to the normal value. The Ps inhibition by CCl_4 in hexane can be decreased drastically by adding C_6F_6 because spur electrons trapped on C_6F_6 can be picked off by the positron while electrons trapped on CCl_4 cannot contribute to Ps formation. In liquid argon where most secondary electrons are thermalized outside the range of the Coulomb attraction the Ps yield is very low. Correspondingly the Ps yield increases very much if molecules which decrease the secondary electron range are added. The strength of the Ps inhibition by "strong" excess electron scavengers correlates with the rate constant of the reaction of the thermalized excess electrons with those scavengers.

The spur process of Ps formation is expected to be important in gases at pressures where spur processes have been shown to be important by radiation chemists. For polyatomic gases this is roughly the case for pressures above approximately 10 atm. The onset of the spur processes probably explains why the ortho-Ps yield increases from 19% to 40% on the increase of the density from 10 amagats to 140 amagats in N_2, for example. Although the application of the spur model on Ps formation in gases have been stressed several times (e.g. by me), it has apparently been mainly neglected until now.

"Aggregation Phenomena in Solutions Studied by

Position Annihilation Technique"

Hans J. Ache

Kernforschungszentrum Karlsruhe GmbH

Institut für Radiochemie

7500 Karlsruhe, Postfach 3640, West-Germany

The study of the positron annihilation process in liquid crystals provided the first evidence that the positron annihilation parameters are not solely controlled by the free volume or changes in the free volume but also by variations in the internal ordering of the molecules, e.g. during mesomorphic phase transitions, where the variation of the available free volume is negligible. Micellization processes are also cooperative, size limited, aggregational processes, which show features similar to classical phase transitions. Positron lifetime measurements in micellar solutions revealed as expected a strong dependence of the annihilation parameters on the type of aggregates formed and can be used to study the composition of these solutions. The work has been extended to reversed micellar solutions, microemulsions and surfactant vesicles. In this progress report the results obtained in these solutions will be discussed and a general outlook on the applicability of the positron annihilation technique for structural studies in these systems will be given.

V.I. Goldanskii and V.P. Shantarovich
Institute of Chemical Physics and Academy of Sciences of
the USSR, 117334 Moscow, Vorobjevskoe Shausse 2b, USSR

We study fluorescene lifetime distributions initiated by single positrons in organic liquids and solids.[1,2] A standard lifetime coincidence system is modified by replacing one detector with a single-photon counter RCA 8850 coupled to a sensitive and fast Timing Filter Amplifier (ORTEC Model 454). When using a ^{22}Na positron source, the delayed coincidnece spectrum between the 1.3MeV positron birth signal and a fluorescence photon gives a measure of recombination rate of electron geminate-ion pairs or the decay of molecular excitation produced in the positron-induced spurs. Such single-particle pulse radiolysis can also be performed with other sources (^{60}Co, ^{90}Sr, ^{210}Po) to study the primary-particle dependence.

We report new results obtained with this method: (1) In hexane and xylol the fluorescence time spectrum of dissolved anthracene is indicative of electron-ion recombination and following deexcitation but not of the decay of direct molecular excitations.[2] (2) In viscous solutions ($\sim$ 10 cp, squalene) both molecular deexcitation ($\sim$ 1 ns) and electron-geminate ion recombination (> 10 ns) are observed.[3] (3) A correlation between the positronium yield and the fluorescence yield was demonstrated through an enhancement of both yields in the presence of a weak electron acceptor ($C_6 F_6$). This effect gives access to the kinetics of some radiation processes.[2,3] (4) If the sample and the source are placed in the resonator of an ESR spectrometor, the ESR spectra of molecular ions can be detected with extremely high sensitivity ($\sim$ 100 ions per sample in steady state) through modulations of delayed photon spectrum.[4,5] This method may elucidate the role of electron trapping by weak acceptors for positronium formation in radiation spurs.

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POSITRONIUM FORMATION AND REACTIONS IN WATER, ICE AND AQUEOUS SOLUTIONS SEEN BY POSITRON AGE-MOMENTUM CORRELATION

Y. Kishimoto and S. Tanigawa
Institute of Materials Science, University of Tsukuba,
Sakura-mura, Ibaraki 305, Japan

Positronium formation has been observed by the narrow peak of the angular correlation curves and I_2 of the lifetime spectra in water, ice and aqueous solutions. In this paper, correlation measurements between positron age and momentum distribution of annihilation pairs were carried out in these systems in order to separate several positronium states. Lifetime spectra were analyzed by two components fitting in each energy channel of Doppler broadning. In every case examined in this work, I_2 can be regarded as a annihilation mode of pick-off process of ortho positronium. The momentum dependence of τ_1 in Fig.1 can be explained as a avaraged lifetime of at least four annihilation modes. Assuming that the momentum distribution for each of these modes is a single Gaussian function, this change of τ_1 occurs when both 1) $\sigma^{(1)} < \sigma^{(2)} < \sigma^{(3)} < \sigma^{(4)}$ and 2) $\tau^{(1)}$ and $\tau^{(3)}$ are shorter than $\tau^{(2)}$ and $\tau^{(4)}$. It seems that two annihilation modes of four, $(\tau^{(1)}, \sigma^{(1)})$ and $(\tau^{(3)}, \sigma^{(3)})$, are the two different states of para positronium. The same tendency as water was observed in ice (Fig.2). But the range of variation of τ_1 in ice was drastically large because of the high probability of positronium formation. The result of aqueous solution containing 3 mol/l of $MnSO_4$ (Fig.3) is probably explained by the efficiency of ortho-para conversion process. Positroniums passing through the conversion process give the longer lifetime than usual para positroniums. It was found that the momentum distribution of such ortho positroniums is narrower than usual self annihilation. This means that initialy formed para positronium are not completely thermalized but converted ones undergo a complete thermalization.
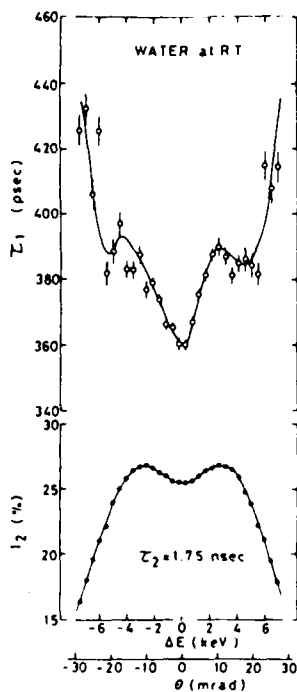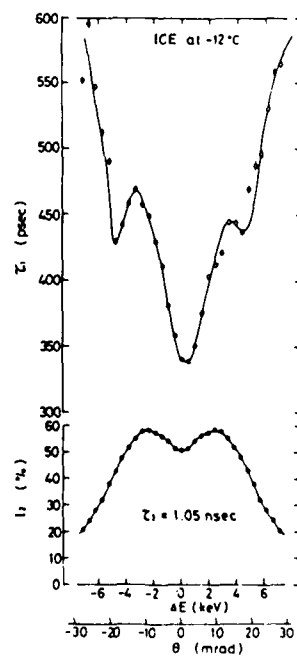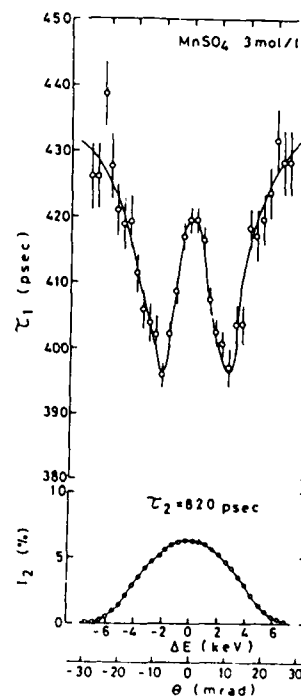
Fig.1   Fig.2   Fig.3

THE TEMPERATURE DEPENDENCE OF ANGULAR CORRELATION CURVES FOR SOLID PIVALIC ACID

P.C. Jain[a], M. Eldrup[b], O.E. Mogensen[b], D. Lightbody[c], and J.N. Sherwood[c].
a) Department of Physics and Astrophysics, University of Delhi, Delhi-11007, India.
b) Chemistry Department, Risø National Laboratory, DK-4000 Roskilde, Denmark.
c) Department of Pure and Applied Chemistry, University of Strathclyde, Glasgow
   G1 1XL, Scotland, UK.

The temperature dependence of angular correlation curves for solid pivalic acid (trimethylacetic acid or 2,2-dimethylpropanoic acid) has been investigated in both its brittle and its plastic phase. All curves are well fitted by a sum of three gaussians, a narrow one (FWHM $\sim$ 3 mrad) and two broader ones (FWHM $\sim$ 8.8 - 9.8 mrad, and 16-22 mrad). The narrow component is associated with the annihilation of para-Ps. Its intensity (I_N) is about 16% in the plastic phase, close to 1/3 of the total ortho-Ps intensity as deduced from lifetimes[1]. Below the solid-solid phase transition ($7°C$) I_N drops to about 9% and then decreases to 0% at $-80°C$ in a sigmoidal manner with decreasing temperature. In this low temperature brittle phase I_N is smaller than 1/3 of the total ortho-Ps yield[1] although the sigmoidal behaviours of the two are very similar. This may be contrasted with the fact that the intensity of a 0.125 nsec lifetime component (normally associated with para-Ps) is higher than 1/3 of the total ortho-Ps yield[1]. Thus the combination of lifetime and angular correlation measurements shows that in the brittle phase of pivalic acid a short-lived (0.1 - 0.2 nsec) positron state must exist or a short-lived Ps state which does not give rise to a narrow angular correlation curve. In the plastic phase on the other hand lifetime and angular correlation data are consistent with the simple picture that only one shortlived state exists, viz. para-Ps the yield of which is 1/3 the total ortho-Ps yield. Ortho-Ps exists in this phase in two different states of which the most long-lived one ($\tau \sim 3$ nsec) is due to ortho-Ps trapped in vacancies (and partly di-vacancies)[1]. From a simple spherical model potential for the vacancy[1] the expected width of the para Ps angular correlation component can be calculated. It comes out in good agreement with the experimental findings. The change in width with temperature of the broad part of the angular correlation curves is well described by assuming it to be a sum of curves representing annihilation of "free" positrons (total FWHM $\sim$ 9.9 mrad) and ortho-Ps pick-off annihilation (total FWHM $\sim$ 9.1 mrad). With increasing temperature the increasing Ps yield gives rise to a narrowing of the total broad part of the angular correlation curve.

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POSITRON ANNIHILATION STUDIES IN
p-NITROBENZYLIDENE-p-n-ALKYLOXYANILINES

P.C. Jain and S.R.S. Kafle[*]
Department of Physics and Astrophysics
University of Delhi, Delhi-110007, India.

Positron annihilation studies have been carried out in four members of a homologous series of p-nitrobenzylidene-p-n-alkyloxanilines. All these compounds exhibit liquid crystalline phase. A study of such series provides useful information about the structure-property relationship. Thermodynamic data for a large number of homologous series has shown some interesting features in this regard. The present work was therefore initiated to see similar effect on the positron annihilation characteristics. In different samples the positron lifetime measurements were carried out as a function of temperature. The time spectrum in each case could be decomposed into two lifetime components. As observed in many other systems, in these compounds also the shorter component, τ_1, showed lesser susceptibility to a phase transition as compared to the longer component, τ_2. The intensity I_2 of the longer component was found to be rather low (⌐ 4%), this could be attributed to the inhibiting action of the nitrogroup in the molecule. In each case the value of τ_2 is found to decrease in going from a phase of higher degree of molecular order to the one having lesser degree of molecular ordering. In this respect the behaviour of these compounds is similar to those of alkyloxy cynobiphenyls. The phase transition temperatures obtained agree with those obtained from differential scanning calorimetry (DSC). These measurements have, however, revealed the existence of a new solid phase in case of p-nitrobenzylidene-p'-n heptyloxyaniline (NBHOA) which has not been observed by DSC. The existence of this new phase has been confirmed by polarized light microscopy. A comparison of the positron annihilation parameters obtained for the different members of the homologous series investigated, does not reveal any definite trend similar to the thermodynamic data. However, in going from an odd member to an even member, the τ_2 value in different phases does show a decreasing trend.

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[*]Presently at the Tribhuvan University, Kathmandu, Nepal.

POSITRON ANNIHILATION STUDIES IN SOME
ALKYL AND ALKYLOXY-CYNOBIPHENYLS

P.C. Jain and C.R.S. Kafle*
Department of Physics and Astrophysics
University of Delhi, Delhi-110007, India

and

V.G. Bhide and B.D. Malhotra+
National Physical Laboratory
Hillside Road, New Delhi-110012, India

Mesomorphic phase transitions in some alkyl-and alkyloxy-cynobiphenyls have been investigated using positron as a probe. All these materials exhibit liquid crystalline phase. In these, the temperature dependence of the positron lifetime was studied. In every case the time spectrum could be decomposed into two components, τ_1 and τ_2. The shorter component τ_1, showed little sensitivity towards a phase transition. Its value exhibited a small change at the solid to smectic/nematic transition and practically no change at the nematic to isotropic liquid transition. As has been reported in many other systems in these compounds also the longer component τ_2, and its intensity I_2 exhibit a greater susceptibility towards a phase transition. In alkylcynobiphenyls the τ_2 value showed an increased in going from solid $\longrightarrow$ smectic/nematic $\longrightarrow$ isotropic liquid phases. Thus in these compounds the τ_2 value in a given phase is found to be strongly correlated with the degree of molecular orientation in that phase, it increases with decreasing degree of molecular order. On the contrary, the alkyloxy cynobiphenyls exhibit an opposite effect. In these compounds the τ_2 value showed a decrease with decreasing degree of molecular order. This difference in behaviour of the two sets of compounds is attributed to the difference in their molecular structures. The present work thus demonstrates that the positron annihilation characteristics are strongly dependent on the nature of inter-molecular interaction.

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*Presently at the Tribhuvan University, Kathmandu Nepal

+Presently at the Department of Applied Chemistry, University of Strathilyde, Glasgow, U.K.

RE-EXAM THE POSITRON LIFETIME ON γ-IRRADIATED ICE SYSTEMS AT 77K

Y. C. Jean*

Department of Physics, University of Missouri-Kansas City
Kansas City, Mo. 64110

J. M. Stadlbauer**, B. W. Ng**, and D. C. Walker**
Department of Chemistry, University of British Columbia,
Vancouver, B.C. V6T1Y6, Canada

Positron lifetimes were measured for the following systems :
(1) polycrystalline ice, 50/50 ice-ethyleneglycol, 10M LiCl-ice, and
1.9M $Cd(ClO_4)_2$ ice at 77K. (2) γ-ray irradiation of above systems
up to 12 MRAD at 77K (3) photobleaching the above postirradiated
systems at 77K. The formation probabilities of trapped Ps
(lifetime 1.1 nsec) are altered due to the photobleaching process.
The correlation between the trapped electrons and the Ps formation
probabilities are discussed in terms of Ps formation mechanisms.

CORRELATION BETWEEN PULSE RADIOLYSIS AND POSITRON ANNIHILATION DATA

J.Ch. Abbé, G. Duplâtre, A.G. Maddock, J. Talamoni, A. Haessler
Université Louis Pasteur et Centre de Recherches Nucléaires
Laboratoire de Chimie Nucléaire
B.P.20, 67037 STRASBOURG Cedex (France)

Measurements have been performed on a wide variety of solutes in aqueous solutions, using both the lifetime spectroscopy and the Doppler broadening of the annihilation radiation line shape techniques. Fitting the data with a limited number of empirical expressions allows parametrization of the inhibiting and of the enhancing capabilities of the solutes towards positronium (Ps) formation.

It is shown that a strong correlation exists between the inhibition constants of the solutes and their rate constants for reaction with the solvated electrons, $k_{(e^-_{aq} + S)}$, as measured in radiolysis experiments, except for a few solutes. Very significantly, most of these abnormal solutes do not follow the Hunt linear relationship between the C_{37} constant (1) and $k_{(e^-_{aq} + S)}$ (2).

A further relevant feature is that some solutes lead to limited inhibition and the Ps intensity plateau values reached at high concentration are the same.

On another hand, it appears that the enhancement parameters are strongly correlated with the rate constants of the solutes for OH scavenging, $k_{(OH + S)}$.

Based on these observations and within the general framework of the spur model (3), a model for Ps formation and inhibition processes is proposed, suggesting two pathways for Ps formation involving either quasifree (dry) or localized (presolvated) particles. This model is discussed with reference to data obtained in other polar solvents (methanol, ethanol, ethyleneglycol) and to the effects of temperature changes. Previous experiments by other authors are critically discussed.

(1) C_{37} is the concentration of solute needed to reduce the solvated electron yield in the pure solvent produced by fast pulse radiolysis to 1/e of its value.

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INHIBITION AND ANTI-INHIBITION EFFECTS

ANALYZED USING RADIATION CHEMISTRY DATA

Yasuo Ito
Tokai Division, Research Center for Nuclear
Science and Technology, University of Tokyo,
Tokai-mura, Ibaraki-ken, 319-11, Japan

Yasuhiro Miyake and Yoneho Tabata
Nuclear Engineering Research Laboratory,
University of Tokyo, Tokai-mura, Ibaraki-ken,
319-11, Japan

The inhibition (by C_2H_5Br and CCl_4) and the anti-inhibition (by C_6F_6) of o-Ps formation in cyclohexane were examined using an emprical equation for the electron scavenging reaction;

$$I(c) = \frac{\sqrt{\alpha\ c}}{1 + \sqrt{\alpha\ c}}$$

which describes the fraction of the scavenged electron in the spur and is well established in radiation chemistry for the electron scavenging reactions in some solvents, cyclohexane being the typical of them.

Assuming that (1) the positron spur is composed of a geminate ion pair (M^+ and e^-) and a positron, and that (2) the above equation can also be used for the electron capture reactions in the spur, the expressions for the inhibition and the anti-inhibition were obtained and were compared to the experimental data.   The agreement was surprisingly well.   It must be emphasized that exactly the same values of the reactivity parameters, α, known in radiation chemistry were used for C_2H_5Br/cyclohexane and C_2H_5Br-C_6F_6/cyclohexane systems.

An additional mechanism of the inhibition other than the electron capture had to be assumed for the case of CCl_4. But once it is assumed the experimental results were also well explained, again using the same values for α as obtained from radiation chemistry, for CCl_4/cyclohexane and CCl_4-C_6F_6/cyclohexane systems.

The present result seems to strongly favor the spur reaction model of Ps formation.   Measurements of the energy spectra of the annihilation radiation support the view that more than one inhibition mechanism is taking place in the case of CCl_4 and suggest that it will involve formation of compounds which contain positrons.

The results of the angular correlation measurements for C_2H_5Br/cyclohexane and CCl_4/cyclohexane systems will also be presented, and discussion will be made to present overall picture of the positron history in the system studied here.

IS THE POSITRON A LIGHT PROTON?   CONTRASTS OF POSITRON/PROTON ANALOGIES IN SMALL MOLECULES

Paul E. Cade and Chih-Mai Kao
Department of Chemistry, University of Massachusetts
Amherst, Massachusetts 01003, U.S.A.

The sequence of positively charged particles, the proton, muon (μ^+), and the positron are identical in basic non-relativistic properties except for their mass. It is thus quite natural to approach the behavior of the muon or positron in their association with a molecule or ion with a reflective view of the parallel behavior of a proton. All three positive particles form a stable system with an electron, H, muonium, and positronium and thus in another vein the 'chemistry' of Ps or Mu might be viewed as parallel, in some respects, that of a hydrogen atom. For example, a proton combines with an OH⁻ to form the very stable HOH molecule and hence one posits that the positive muon would form MuOH and the positron would form PsOH, where the basic 'atoms' involved are written in a parallel fashion, i.e. H, Mu, and Ps. However, it is essential that more than simply the charge state of the system needs consideration in any comparative assessments - the dynamic behavior of the positive particle assumes a vital role. In particular, the Born-Oppenheimer approximation applies only with rather limiting validity. In this paper certain <u>ab initio</u> calculations are presented which shed light on the relationship of the positron to the proton in a parallel set of small molecular ions, i.e. OH⁻, CN⁻, and N₃⁻, which combine with a <u>proton</u> to form the well-known molecules HOH, HCN, and HNNN. The flexibility to consider a positive particle of variable mass (and hence also the muon) is inherent in our calculations.

We report <u>ab initio</u> near Hartree-Fock calculations on the systems [OH⁻:e⁺], [CN⁻:e⁺], and [N₃⁻:e⁺] and here focus on the detailed behavior of the positron in terms of charge density contours. This is part of a study on pseudo-halide ion systems combining with a positron which will be published elsewhere. As Figure 1 shows for the [OH⁻:e⁺] system the positron is localized along the O---H bond axis and at a positron approximately that of another proton in <u>linear</u> water. Attempts to localize the positron, by suitable basis functions, off the axis at the site of a proton in water were rejected by the solution. The implications of these results and similar results for [CN⁻:e⁺] versus HCN and [N₃⁻:e⁺] versus HN₃ are given.
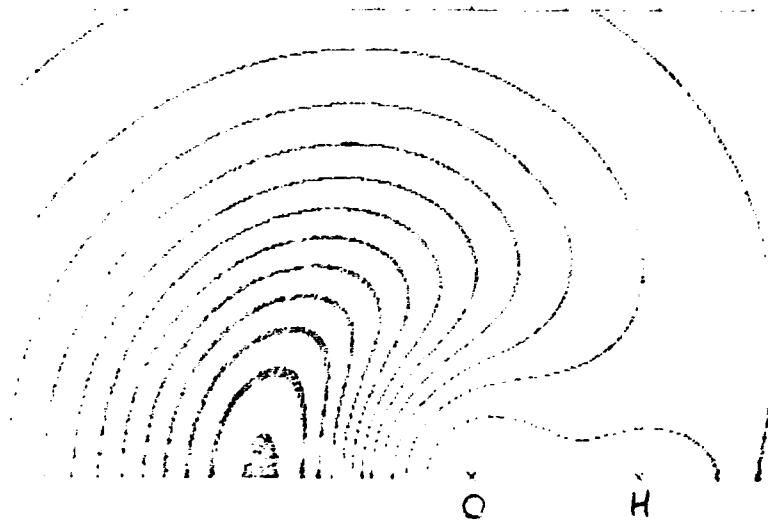
Figure 1.   Charge Density Contours for $\phi_+(\vec{r})$ in [OH⁻;e⁺]

RECOVERY OF DEFORMED AND HYDROGEN-CHARGED PALLADIUM*

C. L. Snead, Jr., K. G. Lynn and J. F. Lynch
Brookhaven National Laboratory
Upton, New York 11973, U.S.A.

Room-temperature lifetime and Doppler-broadening studies have been used to investigate the interaction between interstitial hydrogen and lattice defects in deformed Pd. Two methods of deformation were employed. On the one hand, Pd was cold-rolled to 95% reduction in thickness; on the other, Pd was hydrided to the β phase and then outgassed at room temperature back to the α phase. Hydrogen-containing specimens were then prepared by charging with hydrogen at room temperature to levels of 0.3%. The presence of hydrogen was found to exhibit no effect on the recovery curves of Pd upon annealing to 400°C, leading to the conclusion that traps such as single vacancies are not passivated towards positrons by hydrogen (or that the hydrogen had been released from the traps by the time of the measurement). By 400°C, both specimen sets had recovered to identical levels, but the values for both lifetime and Doppler-broadening were below the values obtained for well-annealed pure Pd. Single-lifetime fits gave values of 120 psec for "well annealed" and 97 psec for 400°C annealed specimens, both cold worked and charged. The fits of the data were comparable but not good. This result is anomalous at this time. Although the specimens hydrided to the β phase and outgassed back to the α phase showed continual recovery up to 400°C, complete recovery was not achieved as with the deformed specimens. The lifetime results indicate the presence of defects larger than single vacancies. One possibility would be the formation of cavities, possibly hydrogen filled, during the hydriding that are stable at 400°C.

A POSITRON STUDY OF NITROGEN DIFFUSION AND CAPTURE BY VOIDS IN Mo

H.E. Hansen, G. Trumpy and K. Petersen
Laboratory of Applied Physics II, Technical University of Denmark
Building 307, DK-2800 Lyngby, Denmark

The pronounced sensitivity of positron lifetime parameters to the capture of nitrogen at voids in Mo was previously reported. Here we present results from investigations of the nitrogen diffusion implantation profile and its dependence of diffusion time, - temperature and voidconcentration. The voidconcentrations were controlled by annealings of neutron irradiated molybdenum single crystals in vacuum ($P < 10^{-8}$ torr). Afterwards the nitrogen was entered by heating at 760 torr in 99.995 % N_2 while taking further precautions for the removal of O_2 and H_2O.

One of the implications of this work is that nitrogen diffusion can be studied at much lower temperatures than previously possible, by using the large positron response to voids and their decoration with nitrogen.

Also the reasons for the positron sensitivity to the nitrogen decoration of the voids are discussed.

THE INTERACTION BETWEEN NITROGEN AND DEFECTS IN
Mo STUDIED BY THE POSITRON ANNIHILATION TECHNIQUE

B. Nielsen, A. van Veen*, L.M. Caspers*, H. Filius*,
H.E. Hansen and K. Petersen

Laboratory of Applied Physics II *Interuniversity Reactor Institute
Technical University of Denmark   Mekelweg 15, Delft
DK-2800 Lyngby, Denmark   The Netherlands

The interaction between nitrogen and vacancies in Mo has been
studied. First interstitial nitrogen was formed in the Mo in a
concentration of $\simeq$ 200 ppm by quenching from 1700°C in a pure
nitrogen gas. Then vacancies were formed by electron irradiation
at $\simeq$ 80°C. The presence of nitrogen caused a strongly increased
vacancy production. The positron lifetime measured after irra-
diation was shorter than for vacancies in pure Mo indicating
that a part of the vacancies are already nitrogen occupied.
Isochronal annealing was then performed. Around 160°C a further
decrease in the positron lifetime was observed. This means
that an increased number of vacancies are nitrogen occupied
and this is most likely due to migration of nitrogen. In the
Stage III recovery region no change was observed, meaning that
no free vacancy migration is taking place, i.e. all vacancies
are nitrogen occupied. The annealing was continued until disso-
ciation of the nitrogen occupied vacancies.

   A Mo single crystal in which nitrogen ($\approx$ 2000 ppm) precipi-
tates were formed after quenching from 900°C in an atmosphere
of 10% N_2 and 90% NH_3, has been studied. The mean lifetime of
positrons in this sample was 140 psec whereas the lifetime in
pure Mo is 120 psec. This effect is attributed to positron
trapping at the precipitates. The interaction between positrons
and precipitates will be discussed. The effect of isochronal
annealing on the precipitates has then been measured.

   The interaction of nitrogen with voids and loops has been
studied by diffusing nitrogen into neutron irradiated Mo. This
was done in an UHV oven under well controlled conditions. The
partial pressure of nitrogen was 10^{-6} torr whereas the partial
pressure of other gasses where below 10^{-9} torr.

THE INTERACTIONS BETWEEN HYDROGEN AND DEFECTS IN METALS STUDIED BY THE POSITRON ANNIHILATION TECHNIQUE

B. Nielsen, A. van Veen*, L.M. Caspers*, W. Lourens*,
G. Trumpy and K. Petersen

Laboratory of Applied Physics II   *Interuniversity Reactor Institute
Technical University of Denmark   Mekelweg 15, Delft
DK-2800 Lyngby, Denmark   The Netherlands

Hydrogen has been injected into Mo containing voids and loops by the use of a small accelerator. The energy, 1.5 keV, was sufficient for penetrating the surface barrier, without causing any damage. After a dose of 2×10^{19} H_2+/cm^2 at $200^{\circ}C$ measurements showed that the number of positrons annihilating trapped in voids have increased $\simeq 10\%$. We interpret this in terms of hydrogen decoration of loops. Isochronal annealing was then performed and it was seen that hydrogen is released from the loops in the temperature region from $300-450^{\circ}C$.

Hydrogen has been electrolytically injected into steels. The presence of hydrogen caused changes in the positron annihilation characteristics. Isochronal annealing has then been performed. The positron annihilation characteristics changed during annealing back to the characteristics measured before hydrogen injection, indicating that hydrogen is annealed out. The positron measurements have been correlated with determinations of the mechanical properties.

Some results on hydrogen electrolytically injected into nickel will be reported.

TEMPERATURE DEPENDENCE OF POSITRON ANNIHILATION PARAMETERS IN NEUTRON IRRADIATED Mo

B. Pagh, H.E. Hansen, B. Nielsen and K. Petersen

Laboratory of Applied Physics II
Technical University of Denmark
DK-2800 Lyngby, Denmark

Abstract

A single crystal molybdenum sample exposed to a neutron irradiation dose of $2.7 \cdot 10^{18}$ fast neutron/cm^2 at $60^{\circ}C$ was annealed at 650, 725, 800 and $875^{\circ}C$ in vacuum ($P < 5 \cdot 10^{-8}$ torr). After the annealings the samples contains vacancy-loops and voids in different concentrations. Lifetime- and Dopplerbroadening measurements were carried out, after each annealing of the sample, in the temperature interval ($-194^{\circ}C$, $285^{\circ}C$). Trapping rates to vacancy-loops and voids were calculated and the possibility of detrapping (escape) of positrons from the vacancy-loops were investigated. It turned out that it is not very likely that detrapping takes place in the above mentioned temperature region.

A brief discussion on diffusion of positrons in molybdenum is given. We found that the temperature dependence of the trapping is governed by that of the trapping tendency i.e. the trapping is transition limited.

A NEW POSITRONIUM-LIKE STATE IN VOIDS IN NEUTRON-IRRADIATED NIOBIUM AND VANADIUM

M. Hasegawa[a], E. Kuramoto[b], K. Kitajima[b], M. Hirabayashi[c],
Y. Ito[d], T. Takeyama[e], H. Takahashi[e] and S. Ohnuki[e]

a) The Oarai Branch, The Research Institute for Iron, Steel and Other Metals,
   Tohoku University, Oarai, Ibaraki 311-13, Japan
b) Research Institute for Applied Mechanics, Kyushu University, Hakozaki,
   Higashi-ku, Fukuoka 812, Japan
c) The Research Institute for Iron, Steel and Other Metals, Tohoku University,
   Sendai 980, Japan
d) Research Center for Nuclear Science and Technology, University of Tokyo,
   Bunkyo-ku, Tokyo 113, Japan
e) Metals Research Institute, Faculty of Engineering, Hokkaido University,
   Sapporo 060, Japan

Many studies on the angular correlation of irradiated metals (Mo, Ni, Al and so on) containing irradiation-induced voids have so far been carried out. Narrowing of the correlation curves by irradiation was observed; reduction of the FWHM was at most 40%. Recent slow positron studies have shown emission of positrons and positroniums from clean surface of metals. It is interesting to study positron state in voids in vanadium-group metals which may have a different surface state from that of other metals.

Niobium and vanadium were irradiated in the JMTR at about 450°C to fluence of $5 \sim 9 \times 10^{20}$ n/cm^2 (>1MeV). The transmission electron microscope observation revealed that the irradiated specimens contained voids of density of about 1×10^{16} cm^{-3}. Diameters of voids were about 30 and 60 Å in niobium and vanadium, respectively.

Fig.1 shows the angular correlation curves for unirradiated and irradiated niobium. A marked narrow component was found in the curves of irradiated vanadium as well as niobium. This component shows emission of positroniums or positrons from void surface to void interior. The gamma-ray energy spectrum did not give any evidence of the 3-γ annihilation. Lifetime-Doppler correlation measurement showed that the narrow component was corresponding to the long lifetime which was close to the spin-averaged lifetime. The results indicate that positrons exists in a positronium state or a free state in voids in niobium and vanadium, and decays primarily by the 2-γ annihilation. Temperature dependence and annealing behavior of the narrow component will be also presented.

Fig.1 Angular correlation curves for the irradiated niobium (9×10^{20}n/cm^2, ~ 420°C) and for unirradiated one.
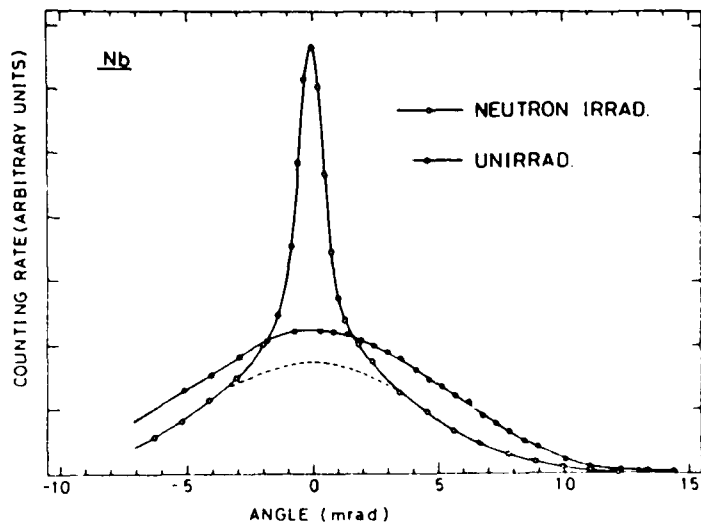
Low-Temperature Positron Lifetimes and Doppler Broadening
Measurements for Single Crystal Nickel Oxide Containing
Cation Vacancies

JAMES T. WABER
        Materials Science and Engineering
        Northwestern University, Evanston, Illinois   60201

KELVIN G. LYNN
        Physics Department
        Brookhaven National Lab, Upton, New York   11973

C. L. SNEAD, JR.
        Metallurgy Department
        Brookhaven National Lab, Upton, New York   11973

Abstract

The lifetimes and Doppler Broadening for positrons anni-
hilating in substoichiometric nickelous oxide have been mea-
sured concomitantly from liquid-helium to room temperature.
The concentration of cation vacancies, as is well documented,
is readily controlled by altering the ambient oxygen pressure
while annealing a single-crystal sample at 1673°K. It was
found that neither of the three lifetimes observed nor their
relative intensities varied significantly with the oxygen
pressure, and the bulk lifetime only increased slightly when
the specimen was cooled from room to liquid-helium tempera-
tures. These results are interpreted as indicating that all
of the positrons are probably trapped by the existing cation
vacancies or have a reduced mobility in annealed crystals.

EVIDENCE FOR SHALLOW POSITRON TRAPS
IN A NEUTRON-IRRADIATED Aℓ SINGLE CRYSTAL

P. J. Schultz and I. K. MacKenzie
Department of Physics, University of Guelph
Guelph, Ontario, Canada
N1G 2W1

K. G. Lynn and C. L. Snead, Jr.
Department of Physics, Brookhaven National Laboratory
Upton, New York, 11973, U. S. A.

R. N. West
School of Mathematics and Physics
University of East Anglia
Norwich, U. K.

A beam of slow positrons has been used to study the dependence on temperature (T ~ 40 to 350 K) of near-surface (<1000 Å) positron diffusion in a single crystal of Aℓ, irradiated by fast neutrons to produce large voids. The results show that the positron diffusion length is proportional to $T^{-\frac{1}{4}}$ above 125 K as would be expected for scattering of the positron by phonons. Below 125 K a severe reduction of this expected diffusion length is observed which we attribute to shallow, radiation-induced traps in the crystal. These results support the conclusions previously reached by Schultz et al for neutron-irradiated Mo.

FUNDAMENTAL INVESTIGATIONS OF POSITRONIUM

D. W. Gidley
Department of Physics, Randall Laboratory
University of Michigan, Ann Arbor, MI 48109, U.S.A.

Richard J. Drachman
Laboratory for Astronomy and Solar Physics
Goddard Space Flight Center, Greenbelt, MD 20771, USA

In the last decade, astrophysics has greatly increased in scope due largely to observations made at previously unobservable electromagnetic wavelengths. Most recently, gamma rays have been detected by instruments on high-altitude balloons and satellites, and these are expected to prove useful in probing the conditions existing in solar flares and near the galactic center.

Among the most interesting of these new discoveries is the unequivocal observation of fairly narrow lines at an energy of 511 keV, evidence of cosmic positron-electron annihilation. These are time-variable, as are the red-shifted lines seen in some of the gamma-ray bursts, whose sources are mostly unknown.

A proper analysis of these types of radiation depends on an understanding of the physics of free positrons interacting with atomic and molecular hydrogen, free electrons and atomic ions. At low enough energies, formation of the positronium atom controls the annihilation process, and the features of the principal reaction,

$$e^+ + H \rightarrow Ps + H^+$$
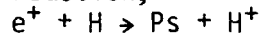
must be computed, since its laboratory realization still lies in the future. The exceedingly low densities obtaining in many astrophysical environments modify greatly the qualitative description of even well-known positron processes.

For example, in the usual high-density laboratory situation positronium formation at an energy above the so-called Ore gap does not lead to annihilation, since the Ps atom is almost certain to be collisionally ionized in a very short time; the positron has simply lost some energy. In space, however, annihilation directly follows Ps formation since mean free times are so long. The typical astrophysical scenario might be described as follows[1,2]: A high-energy positron enters a region containing a mixture of H, H_2, H^- and e^- in proportions depending on temperature, radiation environment and other factors. The positron loses energy by collision, most rapidly if the density of electrons is high. A competition between the Ps-formation rate and the inelastic scattering rate determines the Doppler broadening of the eventual gamma-ray line, while the three-photon annihilation continuum can, in principle, be used to give further information on temperature and ionization fraction in the medium. Interesting plot complications include the possibility[3] of gamma-ray laser action or gravitational red shifts near condensed objects.

The remarkable convergence between advances in the pure atomic theory of positron collisions, the rapid development of elegant experimental techniques, and the recently kindled interest in astrophysical positronics exemplifies nicely the richness of interdisciplinary physics.

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MOTION OF POSITRONIUM IN SOME INSULATING CRYSTALS

K. Fujiwara

Institute of Physics, College of General Education,
University of Tokyo, Komaba, Tokyo 153, Japan

A careful study of the temperature dependence of the momentum distribution of positronium in an insulating crystal is expected to reveal some interesting feature of the dynamic response of such crystallized system of ions or molecules to a foreign, small and light, electrically-neutral composite particle. In this paper, I would briefly describe the recent progress in this field of research achieved mainly by my young co-workers, T. Hyodo, Y. Takakusa and J. Kasai (on Ps in alkali halides), and H. Ikari and S. Tanoue (on Ps in quartz).

The formation of delocalized Ps in insulating crystals was first found in a covalent crystal[1] and later found also in a hydrogen-bonded crystal[2] or in some low-temperature ionic crystals[3]. The discussion about the mechanism of the formation of delocalized Ps in such crystals appears, however, not yet to have been finalized.

An anomalous broadening of the momentum distribution of Ps with increasing temperature was found in quartz, and successfully explained by Ikari[4] as an effect of the damping of the Ps plane-wave states due to Ps-phonon scattering.

A more remarkable, almost dramatic increase with increasing temperature in the width of the momentum distribution of Ps was found far below the room temperature in some alkali halides[5], and interpreted by Hyodo et al.[6] in terms of possible thermal excitation of self-trapped-Ps state situated by 10^{-2} or 10^{-1} eV higher than the bottom of the delocalized-Ps band.

Our preliminary result also shows that the effective mass of Ps is about $3m_e$ in all the materials investigated if Ps is assumed to be thermalized before the annihilation even at lowest temperatures. A more rigorous study of the thermalization and/or effective mass of Ps at low temperatures, however, appears to require a high-resolution one-dimensional angular-correlation machine, and we have not yet performed it at the present stage.

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POSITRON PERCOLATION IN HETEROGENEOUS MEDIA

Werner Brandt
Radiation and Solid State Laboratory
New York University, 4 Washington Place, New York, NY 10003, U.S.A.

POSITRONS IN SEMICONDUCTORS

I. Ya. Dekhtyar

Institute of Metal Physics, Acad.Sci.UkrSSR,Kiev-142, USSR

1. Previously discovered phenomenon of anomalous transition of positrons (ATP) through Si crystals was interpreted in terms of positronium (Ps) formation. Experiments aimed to study the spectra of angular distribution of annihilation photons (ADAP) from Ta have shown that ADAP from polycrystalline Ta with the convertor from Si includes a narrow component (NC) whose half-width corresponds to the thermalized Ps. ADAP from Ta with the use of the Al-convertor has no NC.

2. Microscopic mechanism of ATP assumes Ps quantum diffusion through Si crystal and allows to consider various stages of the process which depend on different temperature dependences of the dif - fusion rate (D). At $T \lesssim \Theta_D$ (the Debay temperature) the mechanism of Ps transition is supposed to be induced by wave vacancies and thus makes it possible to estimate $D_{Ps} \simeq 2.10^{-2} cm^2/sec$ at 300 K.

3. The ATP model takes into account the positron trapping and annihilation as also the Ps formation. Then the total fraction of particles absorbed by the crystal is expressed by the exponential functions from the crystal width, the parameters being dependent on the rate of Ps formation, the velocity of positron trapping and annihilation and a given concentration of trapping centers. The model makes a basis of the absorbtion positron spectroscopy.

4. The convertor from Si was used to study the electronic structure of crystal surface. ADAP from Mo (100) surface was shown to contain a fine structure (FS) which depended on the purity degree. The position of FS elements on the ADAP is determined by the local density of electron states which was calculated for Mo (100).

5. The method of positron spectroscopy of crystal structure defects has been developed. It permits to define the defect distribution by their binding energies with Ps (or positron) in the crystal.

DYNAMIC POSITRON EMISSION TOMOGRAPHY IN MAN
USING SMALL BISMUTH GERMANATE CRYSTALS[*]

Stephen E. Derenzo

Lawrence Berkeley Laboratory and Donner Laboratory
University of California, Berkeley CA 94720, U.S.A.

Primary considerations for the design of positron emission tomographs for medical studies in humans are high imaging sensitivity, whole organ coverage, good spatial resolution, high maximum data rates, adequate spatial sampling with a minimum of mechanical motion, shielding against out of plane activity, pulse height discrimination against scattered photons, and timing discrimination against accidental coincidences. We discuss the choice of detectors, sampling motion, shielding, and electronics to meet these objectives.

TOWARDS HIGH-RESOLUTION POSITRON EMISSION TOMOGRAPHY FOR SMALL VOLUMES

B.T.A. McKee

Metabolic Imaging Research Group
Queen's Univeristy at Kingston, Ontario, K7L 3N6 Canada

The goal of any positron imaging system for medical applications is to produce an image in as short as time as possible which represents as accurately as possible the radionuclide concentration in the target volume. One of the parameters which will affect the accuracy of the reconstructed image is the spatial resolution of the system. However, any efforts to improve the spatial resolution at the expense of overall efficiency will lead to deterioration of accuracy because of statistical fluctuations.

For imaged volume the size of the human head (or larger), the best balance of parameters seems to be provided by an array (usually multiple rings) of scintillation crystals. However for smaller imaged volumes, say 500cc and under, the balance of resolution and efficiency shifts. In order to maintain detail in these smaller volumes high resolution becomes more important and at the same time the requirement for a very large number of coincidence events can be somewhat relaxed.

As a development project at Queen's, we are building a positron imaging system based on the high-density, multi-wire, proportional chamber technology developed by Jeavons at CERN[1]. Our objective is to provide three dimensional imaging capability with spatial resolution of 4 mm x 4 mm x 4 mm in imaged volumes up to 400cc (10cm diameter). This will be used for neurological research with laboratory animals.

The response of our detector system will be described with specific reference to efficiency, spatial resolution, time resolution, and background contribution from Compton scattered and chance-coincidence events.

Three-dimensional image reconstruction for our system will be briefly described with some comments on appropriate representations for three-dimensional images.

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TIME-OF-FLIGHT ASSISTED POSITRON EMISSION TOMOGRAPHY

Nizar Mullani
University of Texas Medical School
Houston, Texas

The incorporation of time-of-flight (TOF) information in a positron camera has been shown to yield improved image quality due to the added information from the localization of the annihilation of the positron. This TOF localization is not sufficient at this time to produce a direct three-dimensional image of an object, but when used in conjunction with a conventional reconstruction process can yield better images containing less noise than was previously possible. With the present cesium fluoride detector technology, a coincidence time below 500 psec FWHM is achievable for an effective gain of a factor or 2 in the signal-to-noise (S/N) ratio. This improved S/N ratio combined with a new technique of utilizing all the interplane cross-coincidence data with TOF positioning can yield effective sensitivity gains by a factor of six over comparable cameras operated in the conventional mode.

The improvement in image signal-to-noise ratio is related to the time-of-flight resolution, object size, intrinsic detector resolution and the reconstructed resolution. Analysis of this mechanism for improvement have shown that for a time-of-flight positron camera the S/N is a function of the ratio of object size to coincidence timing, thereby indicating that maxium count rate yield from time-of-flight imaging occur with large object size such as the human torso.

Design of a clinically useful TOF-PET camera requires optimization of several parameters such as coincidence timing, resolution, scattered radiation, random coincidences and frequency of spatial sampling in order to produce reasonable images. It is also necessary to develop new techniques of data acquisition and image reconstruction for handling the large number of detectors in coincidence and the vast amount of data generated.

There are three time-of-flight systems under construction at this time, one at LETI (France), one at Washington University and one at The University of Texas (Houston). Both the LETI and The Washington University positron cameras utilize 25 mm diameter crystals with intrinsic resolutions of 11.25 mm. The University of Texas system utilizes 18 mm detectors for a resolution of 8.1 mm FWHM. An artists view of The University of Texas TOF PET is shown in Fig. 1.

Figure 1. An artists view of
The University of
Texas Medical School
TOF PET Camera which
is under construction
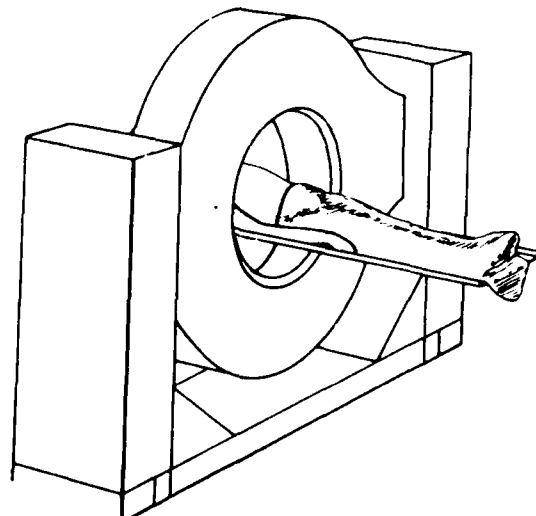
THE HIGH-DENSITY AVALANCHE CHAMBER FOR POSITRON IMAGING

A. Jeavons
CERN, Geneva, Switzerland

and

R. Clack, A. Donath, P. Frey, G. Herlin, K. Hood,
R. Magnanini, D. Townsend
Department of Nuclear Medicine, Cantonal Hospital,
Geneva, Switzerland.

The addition of a high-density drift space to a multiwire proportional chamber has provided a detector for high-energy gamma-rays of high spatial resolution (1 mm) in two dimensions. Pairs of such chambers are now in routine use as positron cameras for angular correlation experiments[1,2] and for medical imaging[3,4].

The development of this type of camera continues at CERN. A new mode of operation has been introduced: using a neon – carbon dioxide gas mixture and a high electric drift-field, electron avalanche multiplication is obtained in the gamma-ray converter. Coincidence time-resolution is reduced to 20 ns and stable chamber operation is achieved with a safe, non-polymerizing gas mixture. This chamber is called a HIgh-Density Avalanche Chamber (HIDAC). Converter construction has been automated using multilayer printed-circuit techniques, enabling chambers with multiple converters to be made relatively cheaply. By this means detection efficiency may be raised from 8% to 25%. To handle the high data-rate from these chambers, the coded centre-of-cluster read-out system has been implemented in hardware.

These developments, and the construction of a large, four-chamber positron camera for medical imaging, will be described.

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POSITRON ANNIHILATION IN ERYTHROCYTE MEMBRANE

S. Y. Chuang and M. E. Ottlinger
Center for Positron Studies, Box 19059, UTA Station,
The University of Texas at Arlington, Arlington, Texas 76019, USA

M. F. Lou
Department of Chemistry
The University of Texas at Arlington, Arlington, Texas 76019, USA

The temperature dependence of positron lifetimes in red blood cell membrane has been studied recently[1]. In this paper, we report our lifetime measurements on ghost membranes which were prepared and then suspended in these conditions: isotonic buffer, hypotonic buffer, and salt free solution (water). Positron lifetimes were measured as a function of temperature from $5^{\circ}C$ to $25^{\circ}C$. For comparison, positron lifetimes in pure water and buffer solutions without membranes were also measured. It was found that positronium pick-off rate (λ_2) shows a sudden change at a temperature near $18^{\circ}C$ for all membrane samples. For other samples without membranes, no sudden change in λ_2 was observed.

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POSITRON STUDIES ON PHASE TRANSITIONS OF
PHOSPHOLIPIDS

Y. C. Jean*

Department of Physics, University of Missouri - Kansas City
Kansas City, Mo.   64110

Positron lifetime measurement has been made on the anhydrous crystalline of DPPC (DL-α-Dipalmitoyl Phosphatidyl Choline) and on the presence of 40% water systems between temperatures 23 and 63°C. The results show that pre-transition and lipid phase transition occur at 35.5 and 41.5°C, which corresponds to the changes of o-ps lifetime and formation probability. The applications of the positron annihilation method to study the phase transition dynamics of biological membranes are discussed.

POSITRON ANNIHILATION STUDIES OF PHASE TRANSITIONS OF FERROELECTRIC, FERROMAGNETIC AND ANTIFERROMAGNETIC CRYSTALS

F. H. Hsu and H. S. Liu
Department of Physics and Astronomy, Georgia State University
Atlanta, Georgia   30303   U.S.A.

E. R. Vance
Materials Research Laboratory, Pennsylvania State University
University Park, Pennsylvania   16802   U.S.A.

Positron annihilation techniques have been widely used for the study of phase transitions in molecular substances and in polymers. In several cases, these techniques have provided new information not revealed by conventional techniques. These investigations were undertaken to determine whether positron annihilation techniques can be used in the study of phase transitions in other groups of materials, namely: ferroelectric, ferromagnetic and antiferromagnetic crystals. We have chosen the following samples: Triglycine Sulfate (ferro-electric), Gd (ferromagnetic) and Cr_2O_3 (antiferromagnetic). The reason for these choices was that the Curie temperatures of the above samples are all easy to reach. Lifetime spectra have been measured in the following tempera-ture ranges: from 260K to 360K for Triglycine Sulfate, from 240K to 340K for Gd and from 250K to 350K for Cr_2O_3. In each case the Curie temperature was in the middle of the range. The temperature dependence of the annihilation spectra was small, but there was definitely a marked change around the Curie temperature for each material.

THE MEASUREMENTS OF THE DOPPLER BROADENING OF POSITRON ANNIHILATION DUE TO THE CDW PHASE TRANSFORMATION IN 1T-TaS$_2$

A.Suzuki , T.Hatano , R.Yamamoto and M.Doyama
Department of Metallurgy and Materials Science , Faculty of
Engineering , The University of Tokyo , Bunkyo-ku Tokyo 113 JAPAN
and
K.Endo , H.Ihara and S.Gonda
Electrotechnical Laboratory , Umezono 1-1-4 Sakura-mura ,
Niihari-gun Ibaraki 305 JAPAN

The layered transition metal dichalcogenide 1T-TaS$_2$ has recently received much attention because of its interesting physical properties which are connected with the formation of charge density wave (CDW).   Especially , 1T-TaS$_2$ is well known by the nearly commensurate-commensurate phase transition at about 200 (K) and transforms into the $\sqrt{13} \times \sqrt{13}$ superlattice.   In order to investigate this CDW transformation from the view point of electronic structure and to get information on the electron momentum distribution , the electrical resistivity , the positron lifetime and the Doppler Broadened lineshape of 511 keV γ-ray emitted   from annihilating positron-electron pairs in 1T-TaS$_2$ were measured in the temperature range between 77 K and 292 K.   The lifetime spectra at room temperature consists of two components , a shorter lifetime T1 (293 psec) which mainly results from the lattice with relative intensity I1 (78 %) and a longer component T2 from the mylar with I2.   Comparing the results with those of other MX$_2$ and MX$_3$,   the structual perfection of the present sample was rather good.   This sample was used for the Doppler Broadening measuraments , where the two crystal directions, "$\parallel$c-axis" (parallel to c axis which is perpendiculer against the layer) and "$\perp$c-axis" (perpendiculer against $\parallel$c-axis) were chosen.   The W-parameters of the Doppler Broadened lineshape were calculated over the temperature range and shown in Figure 1.   Such a simplest parameter can be expected to show the change in the electron momentum distribution due to the formation of the CDW.   Actually the results exhibit a descent around the transition temperature in the direction of $\parallel$ c-axis , which seems to indicate that the nesting of the Fermi Surface occurs at the surface of $\parallel$c-axis direction.   The detailed analysis of the energy spectra by deconvolution will be discussed.

Figure 1.
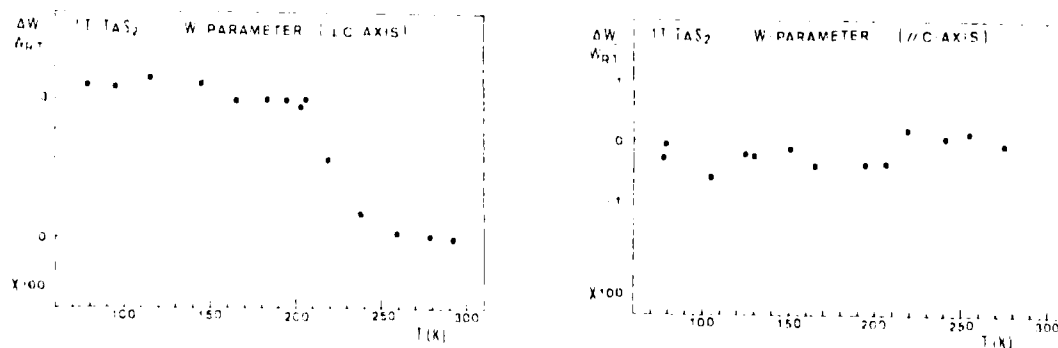
POSITRON LIFETIME AND DOPPLER-BROADENED LINE SHAPE PARAMETERS IN CHEVREL PHASE COMPOUNDS

V. Manohar[+], S. Ramasamy[+], T. Nagarajan[+], C.S. Sundar[++]
K.P. Gopinathan[++], A.M. Umarji[‡] and G.V. Subba Rao[‡]

[+]Department of Nuclear Physics, University of Madras,
A.C.College Campus, Madras 600 025, India.

[++]Reactor Research Centre, Kalpakkam 603 102, India.

[‡]Material Science Research Centre, Indian Institute of
Technology, Madras 600 036, India.

Chevrel phase compounds are of the type $A_x Mo_6 X_8$ (A=metal or vacancy, X=S,Se,Te) possessing high T_c and high H_{c2}. In continuation of our earlier two photon angular correlation results[2], we report, in this paper, positron lifetime measurements and Doppler-broadened line shape parameter(S) in a series of Chevrel phase compounds.

Table 1

Compound	Property and T_c	Lifetime (psec) T_1	Lifetime (psec) T_2	Intensity I_2%
$Mo_6 S_8$	Metal,<1K	223±8	393±3	69±2
$Mo_6 Se_8$	Metal,6.3K	186±3	341±3	52±2
$Mo_2 Re_4 Se_8$	Semicon.	253±2	488±16	7±1
$PbMo_6 S_8$	Metal,15K	206±3	348±4	40±2
$PbMo_6 Se_8$	Metal,3.9K	160±4	311±2	61±2
$Cu_{1.8} Mo_6 S_8$	Metal,10.8K	185±4	348±3	56±2
$Co_2 Mo_6 S_8$	Semicon.	254±1	960±50	2±.2
$Co_2 Mo_6 S_8$	Semicon.	230±3	470±50	4±2[Δ]
$Mo_6 S_6 I_2$	Metal,14K	287±1	760±60	1±.2

[Δ]Data at 77K; all others at 298K

As can be seen from table 1, the data show distinctly two modes of annihilation in the first six compounds and mainly one mode of annihilation in $Mo_6 S_6 I_2$ and $Co_2 Mo_6 S_8$. The trends in T_1 in $A_x Mo_6 X_8$ and $Mo_6 X_8$ (A=Pb,Cu) clearly emphasize the existance of a charge transfer from the A element to the Mo 4d conduction band. The T_2 component in the first six compounds may be attributed to the annihilation in the channel. The electron density (ρ_0) at the annihilation site has been calculated using Brandt's relation. A plot of T_c versus the Fermi angle θ_F (as obtained from ρ_0) for the superconducting Chevrel phase compounds shows an inverse dependence of T_c on θ_F. The structural change in $Co_2 Mo_6 S_8$ at 212K is reflected as a decrease in T_1 and S.

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[2] S.Ramasamy, T.Nagarajan, A.M.Umarji and G.V.Subba Rao,
Phys. Lett. A81, 71 (1981)

[3] W. Brandt, Appl. Phys. 5, 1 (1974)

POSITRON ANNIHILATION PARAMETERS CLOSE TO THE MELTING POINT AND AT PHASE TRANSITIONS

P. Sperr, Quin min Fan[+], and W. Triftshäuser
Hochschule der Bundeswehr München, D-8014 Neubiberg, Germany

High precision positron lifetime and Doppler broadening measurements are performed in metals especially close to their melting points and also at structural transitions. If close to the melting point in metals divacancies are present and play an important role in positron annihilation experiments then characteristic parameters (lifetime and Doppler broadening) should be observed. Materials exhibiting phase transformations (e.g. uranium, iron) show large changes of the Doppler broadening lineshape parameter at these transition temperatures. In order to clarify the role of vacancies at the phase transitions high precision lifetime experiments are being performed.

+ On leave from: Academia Sinica, Peking

THE PRECIPITATION MECHANISM OF Ge IN Al
STUDIED BY POSITRON ANNIHILATION

H.Murakami, I.Kanazawa, T.Kurihara, T.Shimizu and M.Doyama*

Department of Physics, Faculty of Education, Tokyo Gakugei
University, Nukuikitamachi, Koganeishi, Tokyo 184, Japan.
* Department of Metallurgy and Materials Science, Faculty of
Engineering, The University of Tokyo, Kongo, Bunkyoku,
Tokyo 113, Japan.

The precipitation mechanism of alloying elements in
Al-based alloys has been studied by many investigators, and
it has been pointed out that quenched-in vacancies play an
important role during the nucleation and growth of precipitates.
In this study, the positron annihilation technique was applied
to study the nucleation and growth mechanisms of Ge precipi-
tates in Al. The location of vacancies during the precipita-
tion have been made clear.

Specimens, Al-0.2at%Ge, were prepared by melting Al and
Ge with 5 nine purity. They were cold rolled and cut into
dimensions of 20mm x 20mm x 0.5mm. Two pieces were pre-
annealed at 550°C for 6hr, and then quenched from 550°C to
water at 2°C. The ageing time at 2°C was about 5min. They
were aged in an oil bath at temperatures from 50°C to 180°C,
and in an electric furnace from 190°C to 600°C. After each
ageing, two pieces were quenched to water at 2°C. The
measurements of positron annihilation were executed at room
temperature by the Doppler broadening technique by the use of
a Ge(Li) detector. ^{22}NaCl droplet was evapolated on a mylar
foil and sealed with an another mylar foil. This source was
placed between two pieces of specimens. The shapes of Doppler-
broadened lines were characterized by the peak parameter, h
and the side parameter, s.

During the isochronal ageing by the step of 50°C for
60min, s and h parameters decreased from 50°C to 100°C and
then increased to 200°C. They were at constant up to 300°C
and then decreased to 400°C. The initial decrease of
parameters is understood as the evapolation and annihilation
of vacancies trapped by clusters of Ge atoms which were formed
during or just after the quenching. The aggregates of Ge
atoms and vacancies may be in small size since the vacancy
evapolation takes place by the ageing at temperatures below
100°C. The decrease of s and h parameters during the ageing
at 50 - 100°C is the direct evidence of the trapping of
vacancies by the nuclei of Ge precipitates. The following
increase and decrease correspond to the growth of precipitates
and the dissolution of precipitates, respectively. These
change of parameters show that positrons are trapped by Ge
precipitates.

THE RECOVERY OF QUENCHED Al-Sn ALLOYS
STUDIED BY THE POSITRON ANNIHILATION

I.Kanazawa, H.Murakami, T.Kusuka, Y.Sakurai and M.Doyama*

Department of Physics, Faculty of Education, Tokyo Gakugei
University, Nukuikitamachi, Koganeishi, Tokyo 184, Japan.
* Department of Metallurgy and Materials Science, Faculty of
Engineering, The University of Tokyo, Hongo, Bunkyoku,
Tokyo 113, Japan

It is interesting to study the recovery of quenched
Al-Sn alloys since the high binding energy of a vacancy-Sn
atom pair, about 0.4eV, is usually accepted. From this point
of view, the recovery of quenched-in vacancies in Al-Sn
alloys has been studied by the positron annihilation
technique. Specimens, Al-50ppmSn, were prepared by melting
Al and Sn with 5 nine purity. They were cold rolled and cut
into dimensions of 0.5mm x 15mmϕ. ^{22}NaCl droplet of
approximately 10μCi was evapolated on a specimen surface and
sealed with the other specimen. They were annealed at 550°C
for about 6hr and quenched to methyl alcohol at -90°C. The
isochronal annealing treatments were carried out by the oil
bath in the temperature range from 0°C to 150°C. The tempe-
rature of specimen was kept at -196°C during the measurement
of positron annihilation. The shapes of Doppler-broadened
lines were characterized by the peak parameter, h, and the
side parameter, s.

During the isochronal annealing by the step of 10°C for
10min, s parameters slightly increased from the as-quenched
state to 0°C, decreased to 60°C and increased from 60°C to
100°C. They were nearly constant from 100°C to 130°C and
then decreased to 150°C. The quenching rate was low since
the specimen thickness was 1mm. Therefore the pairs of a
vacancy-Sn atom were already introduced in the specimen just
after the quenching. The slight increase by the ageing at
0°C may correspond to the clustering of some part of a
vacancy-Sn atom pairs. The following decrease of parameters
to 60°C shows the break-away and annihilation of vacancies
from a vacancy-Sn atom pairs and from small clusters of
vacancies-Sn atoms. The increase of parameters from 60°C
to 100°C is understood as the growth of Sn precipitates.
The decrease of parameters by the annealing above 130°C
corresponds to the annihilation of secondary defects such
as vacancy loops and voids. Experiments in more detail are
now in progressing.

POSITRON ANNIHILATION IN AL-0.55 at.% Mn

T. Troev and P. Topalov[*]
Institute of Nuclear Research and Nuclear Energy,
Sofia-1184, Bulgaria
*Physics Department of the Sofia University, Sofia-1126, Bulgaria

In the recent years the possibility for using positron annihilation for investigating the influence of different factors on structure of solids was shown in a number of works. Positrons in solids can be trapped by the formed defects around which the positrons possess unique annihilation characteristics.

In the present paper the annihilation of positrons in Al containing 0.55 at.% Mn has been investigated experimentally aimed at fixing the influence caused by the recrystallization temperature upon on the curves of the angular correlation and the shape of the energy spectrum of the annihilation gamma-quanta. Doppler broadening and angular correlation were measured versus quenching temperature up to 320°C. It is observed a slight change in the intensity of parabolic component and H-parameter of DBAGL in the temperature range from 20°C to 198°C. The recrystallization effect in Al-0.55 at.% Mn influence the annihilation rate in the temperatures around 230°C. During quenching at those temperatures are formed complex of vacancy-impurity atoms. Above 230°C the increasing of the annihilation rate of positrons due to new distribution of electrons. The measurements of coincidence counting rate in the peak of the angular correlation curve:

$$h = \frac{N_{(P_z=0)}}{N_{(p_z)}\, dp_z}$$

show a considerable difference between quenched and heated specimen for the temperatures around 230°C.
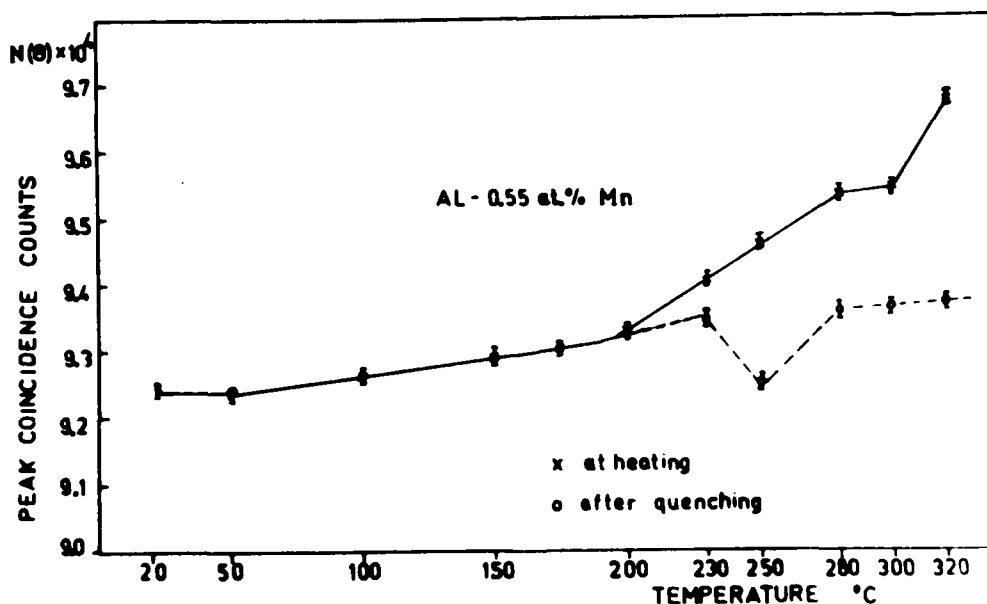
POSITRON STUDIES OF SOLUTE CLUSTERING
AND LATTICE DEFECTS IN Al-Zn ALLOYS

A. Alam and R. N. West
School of Mathematics and Physics
University of East Anglia, Norwich, England.

It is well known that in low concentration Al-Zn alloys there is a tendency for the Zn atoms to cluster. It also appears that Zn atoms in aluminium have a higher positron affinity than the host atoms. This and the additional fact that many positron annihilation parameters for the two metals are significantly different make the Al-Zn system a particularly apt choice for positron studies of clustering phenomena.

In this paper we report studies of the annealing behaviour of samples initially quenched from 0.9 Tm to 200K or room temperature or heavily deformed at room temperature or at 77K.

The measured annealing curves provide clear evidence of positron trapping at both open volume defects and at Zn-rich clusters and their analysis provides insight into the formation and dissolution phenomena.

A POSITRON STUDY OF PRECIPITATION PROCESSES IN AGE-HARDENABLE Al-Zn ALLOYS WITH ADDITIONS OF Mg OR Ge

G. Dlubek, O. BRÜMMER, and R. Krause
Sektion Physik der Martin-Luther-Universität Halle-Wittenberg
DDR-4020 Halle (Saale), Friedemann-Bach-Platz 6
German Democratic Republic

Recently, it was shown by positron lifetime, annihilation lineshape and angular correlation measurements that positrons are strongly localized at Zn-rich Guinier-Preston (GP) zones in Al-Zn alloys /1, 2/. In alloys having a Zn content of 4,5 % or more positrons are almost completely trapped by GP zones after ageing of quenched samples at room temperature. In that case, the Zn content of GP zones was determined to amount (69 ± 5)at. %. After quenching the alloys from 570K in methanol at 200K positrons are trapped by both, vacancies and GP zones. The recovery of vacancies as well as the growth of zones were observed /2/. Above room temperature the well-developed zones are free of vacancy-type defects. The dissolution of GPzones was observed to occur above 100 °C /1/.

Small Mg additions, such like 0,2 at. %, modify strongly the positron results which are interpreted in terms of positron trapping by monovacancies bound to Mg atoms <u>inside</u> the Zn-rich GPzones /3,4/. Further, indications of positron localization at incoherent parts of the interfaces results were supported by small angle X-ray scattering and transmission electronmicroscope investigation /1,3/.

The aim of the present work is to compare the effects of Mg or Ge additions on the behaviour of vacancies in Al-Zn alloys. The positron results are interpreted in the following way. Both elements, Mg and Ge, trap quenched-in vacancies after room temperature ageing of samples. Positrons are localized at Reese complexes. The vac-Ge complexes are distributed over the matrix independently of the Zn-rich GP zones. An alternative trapping model is formulated for Al-Zn-Mg which assumes vacancy-type positron traps inside GP zone traps. The data simulation helps in a more quantitative interpretation of measured results.

/1/   G. Dlubek, O. Kabisch, O. Brümmer, and H. Löffler
      phys. stat. sol. (a) <u>55</u>, 509 (1979)

/2/   G. Dlubek, O. Brümmer, J. Yli-Kauppila, and P. Hautojärvi,
      J. Phys. F., in press

/3/   O. Kabisch, G. Dlubek, H. Löffler, O. Brümmer, and R. Gerlach,
      phys. stat. sol. (a), <u>59</u>, 731 (1980)

/4/   G. Dlubek, O. Brümmer, P. Hautojärvi, and J. Yli-Kauppila,
      Phil. Mag. A <u>44</u>, 239 (1981)

IMPURITY EFFECTS ON THE FORMATION OF DIVACANCIES IN ALUMINUM OBSERVED BY THERMAL EQUILIBRIUM MEASUREMENTS OF ANNIHILATIJN LINESHAPES

S. Tanigawa, K. Ito, Y. Ohtsu and K. Shima
Institute of Materials Science, University of Tsukuba,
Sakura-mura, Ibaraki 305, Japan

Thermal equilibrium measurements of Doppler broadening of annihilation radiations have been applied to a series of dilute aluminum based alloys.   In Fig.1, the lineshape parameters of 99.999% pure aluminum are plotted as a specimen temperature.   This temperature dependence is common one to many other metals and can be explained by two states (free and trapped states at vacancies) trapping model.   In the present paper, however, it was found that the addition of a small amount of impurity atoms induces a drastic change in temperature dependence. In Figs. 2, 3, 4, 5 and 6, the results of Al-0.5at.%Li, Al-0.5at.%Mg, Al-0.03at.% Cu, Al-0.08at.%Ag and Al-0.8at.%Ca alloys are shown respectively.   In dilute alloys, the threshold temperature for the onset of vacancy effects shifted to lower temperatures.   Furthermore, the lineshape parameter abruptly increased towards the melting point.   The former effect can be attributed to the formation of vacancy-impurity atom pairs, and the latter to the formation of divacancy-impurity complexes.   These phenomena were successfully analyzed by the four states (free state, trapped states at single vacancies, vacancy-impurity atom pairs and divacancy-impurity atom pairs, respectively) trapping model.   Derived values of the binding energies both between a single vacancy and a solute atom and between a divacancy and a solute atom will be presented at the conference.   In order to check this phenomenon more precisely, experiments on other systems, Al(Sn), Al(V), Al(Ge), Al(Si) and Al(Zn) are now in progre s.   In addition, thermal equilibrium measurements of positron lifetimes are planned.
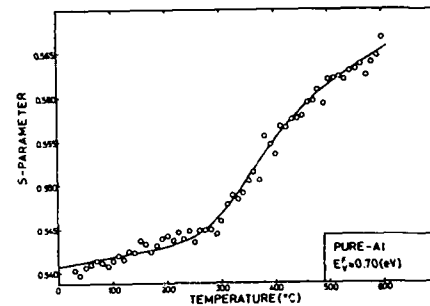
Fig. 1
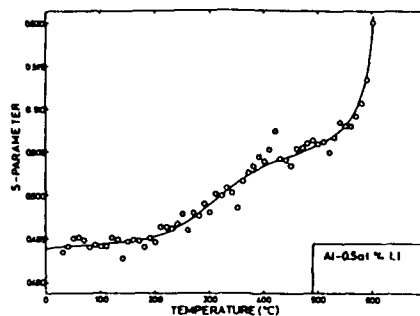
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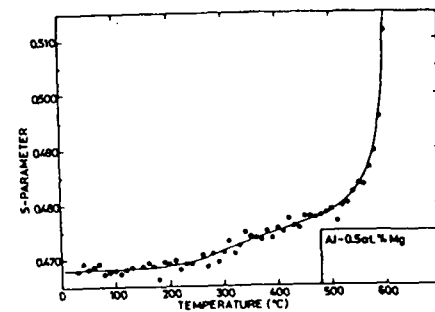
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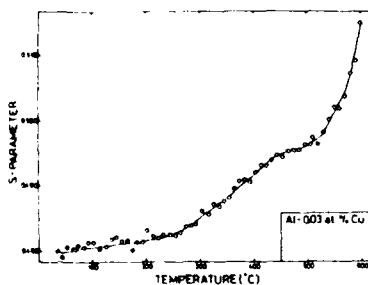
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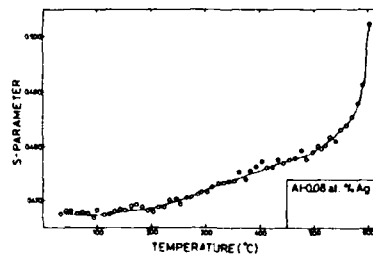
Fig. 5
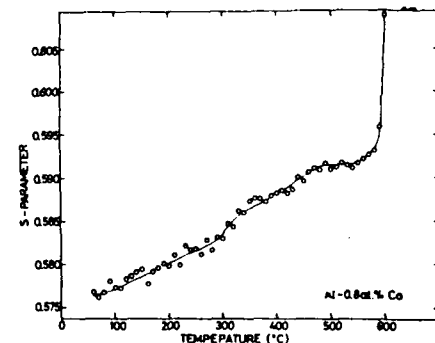
Fig. 6

STUDIES OF QUENCHED-IN DEFECTS AND THEIR RECOVERY IN SINGLE CRYSTALS OF Al, Al-1.5 x 10^{-2} at% Mn, Al-3 x 10^{-2} at% In, Al-1.0 x 10^{-2} at% Si AND Au BY POSITRON ANNIHILATION SPECTROSCOPY

G.M. Hood and R.J. Schultz
Atomic Energy of Canada Limited, Chalk River Nuclear Laboratories,
Chalk River, Ontario, Canada   K0J 1J0

Single crystals of Al, Al-1.5 x 10^{-2} at% Mn, Al-3 x 10^{-2} at% In, Al 1.0 x 10^{-2} at% Si and Au have been quenched from elevated temperatures and the quenched-in defect structures and their recovery studied by positron annihilation spectroscopy – using the Doppler-broadening technique. The results are presented in terms of lineshape parameters, S and W, based on relative areas within well-defined energy intervals at the peak and in the wings, respectively, of normalized annihilation photopeak spectra.

The quench temperatures were 753 K for pure Al and the Mn and In alloys, 859 K for the Al(Si) alloy and 123 K for the Au samples. In the as-quenched state, prior to recovery, S has a clear, positive temperature dependence for Al, Al(Mn), Al(In) and Al(Si); neither the S nor W data for quenched Au, nor the W data for quenched Al, Al(Mn) and Al(In) permit a clear assignment of a temperature dependent form. Preliminary results for the Al(Si) alloy show that a relatively strong and reversible temperature dependence of S and W also exists after the early stages of sample annealing.

The recovery spectra for Al, Al(Mn) and Al(Si) show that major changes in the defect structures occur in the intervals 200-300 K and 380-480 K; between 200 and 250 K an increase in the value of S – particularly evident for the alloys – is associated with the formation of vacancy aggregates, the value of S then declines, exhibiting a plateau-like region from $\sim$ 300-380 K. In this last region the value of S for the Si alloy is much enhanced compared to the Al and Al(Mn) results. Final recovery towards the fully-annealed-state parameters occurs in the range 380-500 K. In all of these materials the recovery of W is made conspicuous by the relative absence of a strong change in the defect signal – to parallel the increase in S – in the early stages of defect recovery. The recovery characteristics for the Al(In) alloy are quite distinct from those of the other Al-based specimens. Neither S nor W displays significant annealing effects below 260 K; W displays strong recovery in the interval 280-400 K, at the end of which interval super-recovery is evident, the major recovery of S occurs in the range 320-400 K. From 400-500 K, W decreases back towards its annealed state value while in the same interval S exhibits a humped recovery profile with a peak at 450 K, by 550 K both S and W are close to their fully annealed state values.

The bulk of recovery for the quenched Au lies in the intervals 300-420 K and 750-940 K. The recovery in the lower temperature range is apparently quite complex.

POSITRON LOCALIZATION IN ALUMINIUM ALLOYS

F. Boileau, B. Geffroy, R. Paulin
Centre d'Etudes Nucléaires de Saclay, Service INSTN
91191 Gif sur Yvette cedex, France

Lifetime, angular correlation and Döppler data relative to positron annihilation in eight aluminium alloys $\left(\text{AlMg}_{0.1\%,\ 1\%, 11\%}\ ,\ \text{AlZn}_{2\%,\ 7\%},\ \text{AlCu}_{4\%}\ ,\ \text{AlAg}_{1.2\%}\ ,\ \text{AlGe}_{2\%}\right)$ are analysed in terms of positron trapping by vacancies bound to impurities and/or by impurity enriched zones.

From isochronal and isothermal annealing experiments in quenched AlMg alloys the dynamic behaviour of two different vacancy-impurity complexes are resolved. Their migration energy is measured to be 0.8 ± 0.1 eV and 0.9 ± 0.05 eV.

The dynamic of impurity clustering is studied in AlZn, AlAg, AlMg, AlCu and AlGe from annihilation parameters indicating a preferential localization of positron in zone enriched with impurities. The threshold of positron sensitivity to various precipitation processes is estimated and the relative magnitude of positron affinity to various metals is compared to the theoretical predictions [1, 2].

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POSITRON STUDIES OF AMORPHOUS METALLIC ALLOYS

N. Shiotani
The Institute of Physical and Chemical Research
Wakoshi, Saitama 351, Japan

Amorphous metallic alloys are metastable solids with atomic arrangements which are not spatially periodic. Although nominally pure elemental amorphous metals can be prepared, most of them crystallize well below room temperature. Therefore current studies are limited to those on amorphous alloys which can be retained, at least, at room temperature. Amorphous alloys are produced in a variety of ways; evaporation, sputtering and electro and chemical deposition, as well as quenching from the liquid state. The amorphous alloys currently studied may be classified conventionally into four groups according to their constituents; 1) transition or noble metal-metalloid (Pd-Si, Fe-B etc.), 2) transition metal-noble metal (Zr-Cu, Ti-Cu etc.), 3) rare earth-transition metal (Gd-Co, Gd-Ni etc.), 4) simple metal-simple metal (Mg-Zn, Ca-Mg etc.).

There is one fundamental difference between studies of crystalline solids and those of amorphous solids. For crystalline solids three-dimensional atomic structure can be determined experimentally by X-ray, neutron or electron diffraction. Therefore, we can discuss various properties of them on the basis of the experimentally determined atomic structure without asking why that structure should be realized under the given conditions (composition, temperature, pressure etc.). On the other hand, for amorphous solids the three-dimensional description of atomic arrangements cannot be uniquely given experimentally. Only one-dimensional average radial distribution of atoms can be determined by X-ray, neutron or electron scattering. Therefore, we have to start by constructing a model of three-dimensional atomic arrangements. Then we discuss their various properties on the basis of that constructed model. Furthermore, since the amorphous solids are metastable, i.e. not in thermal equilibrium, the microscopic atomic structure of one specimen may differ from that of another specimen of the same composition. It has been known that some properties of the amorphous alloys depend strongly on the history of the specimen.

In general, the state of the positrons in matter is determined by the atomic structure and the electron distribution in that atomic structure. Thus, it is expected that measuring the annihilation characteristics gives us information on the atomic and electronic structure of matters. However, interpretation of measured annihilation characteristics becomes very difficult when we do not know either of the atomic and electronic structures and the positron state exactly. This is the situation we are in for the study of positron annihilation in amorphous alloys.

In this talk the positron studies of amorphous alloys published in these years will be reviewed. The atomic and electronic structures, the structural relaxation, the crystallization processes of amorphous alloys will be discussed in connection with the annihilation characteristics.

POSITRON ANNIHILATION IN LAYERED STRUCTURES

F. Heinrich and E. Cartier
Laboratory of Solid State Physics, Swiss Federal Institute of Technology ETH
CH-8093 Zürich, Switzerland

P. Pfluger and H.-J. Güntherodt
Institut für Physik, Universität Basel
CH-4056 Basel, Switzerland

As a very characteristic example for positron annihilation in layered structures, experimental results obtained with graphite intercalation compounds (GIC's) are summarized. GIC's form ordered sequences of graphite and intercalated layers. In many cases they can be prepared in different "stages". The stage number n is defined as the number of carbon planes between two successive intercalated layers. A large variety of atomic and molecular species can be intercalated. According to the nature of the intercalant, GIC's can be divided into two groups: Donor compounds containing metallic intercalants such as alkali metals, Ca, Eu and acceptor compounds produced by intercalation of molecular species as Cl_2, Br_2, ICl, $AlBr_3$, SbF_5 and others. Such broad possibilities to "manipulate" GIC's together with the remarkable anisotropy of their electronic properties (two-dimensional synthetic metals) make GIC's most attractive for angular correlation experiments.

The observed positron annihilation characteristics differ drastically for acceptor- and donor-intercalated graphite.

In acceptor GIC's the angular correlation distributions are independent of n and differ significantly from that observed in pure graphite. This behavior can be explained by the formation of quasi-free positronium complexes within the intercalated layers. For simple acceptor species (Br_2, Cl_2) the experimental angular correlation distributions are dominated by annihilations from positron-halide-states as $[Br^-; e^+]$, $[Cl^- ; e^+]$ as calculated by Farazdel and Cade [1]. For more complex intercalants, the intercalation chemistry is not very well known. Nevertheless, in some cases positron experiments offer a welcome possibility to identify the anionic species within the intercalant.

In donor compounds the positron is repelled from the positively charged intercalant layer. The drastic n-dependence of this effect helps to yield information on the charge distribution of higher stage potassium intercalated graphite. The results of n = 1 donor compounds are discussed in terms of existing bandstructure calculations.

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INVITED PAPER
(Title to be announced)

B. Rozenfeld
Institute of Experimental Physics
University of Wroclaw, 50-205 Wroclaw, Poland

ANNIHILATION PARAMETERS IN METALS AT LOW TEMPERATURES

I. K. Mackenzie
Physics Department, University of Guelph
Guelph, Ontario, N1G 2W1, Canada

VACANCY-LIKE DEFECTS IN IRRADIATED
AMORPHOUS ALLOYS

P. Moser, P. Hautojärvi[*], J. Yli-Kauppila[*], C. Corbel[**]
Centre d'Etudes Nucléaires de Grenoble
Département de Recherche Fondamentale
Section de Physique du Solide
85 X - 38041 GRENOBLE CEDEX, France

Positron lifetime technique is used to study vacancy-like defects in amorphous alloys of $Fe_{80}B_{20}$, $Fe_{40}Ni_{40}P_{14}B_6$, $Pd_{80}Si_{20}$ and $Cu_{50}Ti_{50}$.

In the as-received state the lifetime values (142, 147, 155 and 159 psec, respectively) are typically intermediate between those for well-annealed and defected metal constituents of the alloys. This is interpreted as positron trapping at pre-existing holes smaller than one atomic volume. Weak hydrogen doping does not seem to change the positron lifetime values.

Low temperature electron irradiation is found to increase the positron lifetime to a level close to the values for monovacancies in crystalline metals. Thus irradiation induces vacancy-like defects, which are capable of trapping positrons. The defects anneal out continuously without any visible stages from 77 K to 300 K and at room temperature practically no marks of radiation damage are observed. No evidence of clustering of the irradiation-induced defects are found. Instead, after a high-dose electron irradiation, as well as after neutron irradiations, positron lifetimes shorter than those in the as-received state of the alloys are measured after heat-treatments around room temperature. This is explained by irradiation-induced crystallization seen also in X-ray measurements.

The properties of the irradiation-induced defects are discussed in analogy with the "close Frenkel pairs" of crystalline metals. The size of the vacancy-like defect is about the size of the knocked-on atom, which stops close to the vacancy and remains in a strong elastic interaction with it. The annealing of the pair occurs by thermally activated collapse. The continuous recovery suggests a wide range of pair configurations.

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*   Laboratory of Physics, Helsinki University of Technology, 02150 Espoo 15, Finland
** Section d'Etudes des Solides Irradiés, Centre d'Etudes Nucléaires de Fontenay-aux-Roses, BP6 92260 Fontenay-aux-Roses

INVESTIGATION OF VACANCY-LIKE DEFECTS IN AMORPHOUS METALS BY POSITRON ANNIHILATION

G. Kögel and W. Triftshäuser

Hochschule der Bundeswehr München, D-8014 Neubiberg, Germany

Amorphous metals have been investigated by various methods of positron annihilation (lifetime, Doppler broadening, slow positrons). Both intrinsic and radiation induced defects have been found.

In amorphous metal - metalloid alloys (metal: Fe, Ni, Co; metalloid: B, Si,P) positrons are always trapped at vacancy-like intrinsic defects. This conclusion is based on the following results:

1. The positron annihilation parameters in the amorphous alloys are very similar to the ones obtained for dislocations in the corresponding deformed crystalline metals. However, they differ markedly from those in the annealed crystalline metals and alloys.

2. The temperature dependence of the annihilation parameters is 4 to 7 times larger compared to the crystalline state. From this dependence a distribution of binding energies from 0.1 to 0.3 eV is derived.

3. The positron diffusion length in amorphous metal-metalloid alloys is of the order of $100\overset{\circ}{A}$, in contrast to the crystalline metals where the positron diffusion length is typically $1000\overset{\circ}{A}$. A total defect concentration in the range of 0.1 at% to 1 at% is estimated from this difference.

Also radiation induced defects have been observed in amorphous metals.

In $Ni_{76} Si_{12} B_{12}$ a heavily damaged layer has been created by irradiation with α-particles of 8 keV at about 300K. The evolution and the recovery of this defect layer are studied up to 500K.

In $Ti_{50} Be_{40} Zr_{10}$ irradiation with electrons of 1.5 MeV at 80K introduces a distinctive defect state with a lifetime of 250 psec. Continuous recovery of this defect without marked recovery stages is observed from 100K to 300K.

TEMPERATURE DEPENDENCE OF POSITRON ANNIHILATION PARAMETERS IN METALLIC GLASSES $Fe_{40}Ni_{40}P_{14}B_6$ AND $Fe_{40}Ni_{38}Mo_4B_{18}$

C.S. Sundar, A. Bharathi and K.P. Gopinathan

Reactor Research Centre, Kalpakkam 603 102, Tamil Nadu, India

Positron lifetime measurements have been made in $Fe_{40}Ni_{40}P_{14}B_6$ and $Fe_{40}Ni_{38}Mo_4B_{18}$ metallic glasses at 298 K and 77 K. The mean lifetime values are : τ = 168 $\pm$ 2 psec at 298 K and 165 $\pm$ 2 psec at 77 K in $Fe_{40}Ni_{40}P_{14}B_6$ and 156 $\pm$ 2 psec at 298 K and 155 $\pm$ 2 psec at 77 K in $Fe_{40}Ni_{38}Mo_4B_{18}$. Doppler broadened lineshape parameters have been measured as a function of temperature from 10 K to 298 K in $Fe_{40}Ni_{40}P_{14}B_6$ with values varying from I = 0.515 $\pm$ 0.001 at 10 K to I = 0.521 $\pm$ 0.001 at 298 K. The lineshape parameter in $Fe_{40}Ni_{38}Mo_4B_{18}$ varies from I = 0.521 $\pm$ 0.001 at 77 K to 0.525 $\pm$ 0.001 at 298 K. The variation of the lineshape parameter with temperature is analogous to that in metals containing voids, eventhough the magnitude of variation is much smaller. Because of the larger experimental errors in the lifetime values variation of a few percent could not be established with certainty in lifetime values. The results indicate the presence of vacancy-like defects in metallic glasses.

The influence of production process on imperfection structure of metallic glasses as seen by positron annihilation investigations

Zs. Kajcsos, L. Marczis[+], A. Lovas, Cs. Szeles, D. Kiss, G. Brauer[*]

Central Research Institute for Physics
H-1525 Budapest, P.O.B. 49, Hungary
[+]Research Institute for Ferrous Metallurgy
H-1509 Budapest, P.O.B. 14, Hungary
[*]Zentralinsitut für Kernforschung Rossendorf
DDR-8051 Dresden, pf. 19., GDR

Positron annihilation investigations were carried out on Fe-Ni-based amorphous metallic alloys produced by the spinning-wheel method. The samples were prepared applying different cooling rates. Both positron lifetime data and results of measurements of the Doppler-broadening have revealed the presence of trapping centres in the amorphous phase; a correlation was found between the size+concentration of these positron-active structural imperfections and production parameters. The results clearly indicate the usefulness of positron annihilation measurements for the study of amorphous metallic alloys.

ELECTRON MOMENTUM DENSITIES IN Nb-Mo ALLOYS

Y. Nakao and S. Wakoh*
Department of Physics, Aoyama Gakuin University,
Chitosedai, Setagaya-ku, Tokyo 157, Japan
*University of Library and Information Science,
Yatabemachi, Tsukubagun, Ibaraki 305, Japan

The electron momentum densities in Nb-Mo binary alloys are calculated on the basis of the ATA scheme proposed by Mijnarends and Bansil.[1] Both niobium and molybdenum are paramagnetic transition metals having body centered cubic structure and these characters remain in $Nb_{1-x}Mo_x$ systems throughout whole concentration range. The electronic band structures of niobium and molybdenum have found to be essentially same. The positron annihilation and the Compton scattering experiments should be valuable tools for studies of the band structure and the geometry of the Fermi surfaces as well as the electron momentum density in concentrated disordered alloys. Calculations of the band structure of Nb-Mo systems have been reported by Colavita et al.[2] based on the CPA scheme and by the present authors[3] based on the ATA scheme. Recently, two-dimensional angular correlations of Nb-Mo alloys have been obtained by West.[4]

For calculations of the band structures of disordered alloys, construction of a proper alloy potential is essential. We construct the alloy potential for Nb-Mo system, by starting from the muffin-tin potentials of pure niobium and pure molybdenum. In order to take into consideration charge transfer between the constituents in $Nb_{1-x}Mo_x$, the muffin-tin potential of pure niobium is shifted by an amount $E_F^{Nb}-\bar{E}_F$ and that of pure molybdenum by an amount $E_F^{Mo}-\bar{E}_F$, here, $\bar{E}_F=(1-x)E_F^{Nb}+xE_F^{Mo}$. A part of calculated momentum density spectrum is shown in Fig.1 for x=0.5 in arbitrary units. The calculated two-dimensional electron momentum densities will be presented and compared with the experimental results by West.[4]
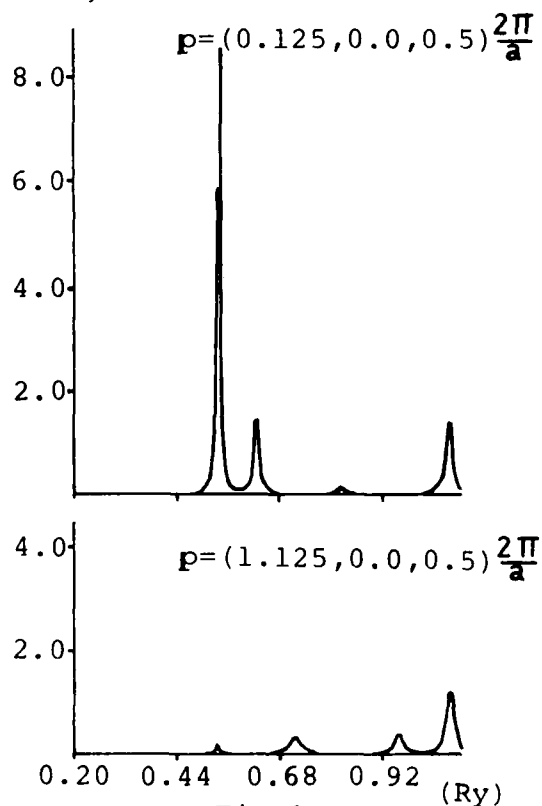
Fig.1

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EXPERIMENTAL AND THEORETICAL STUDY OF THE ELECTRONIC STRUCTURE OF $Co_{0.92}Fe_{0.08}$
BY POLARIZED POSITRON ANNIHILATION AND ANGLE-RESOLVED PHOTOEMISSION

L.P.L.M. Rabou, P.E. Mijnarends
Netherlands Energy Research Foundation ECN, Postbus 1,
1755 ZG Petten, The Netherlands
H. Neddermeyer
Institut für Experimentalphysik der Ruhr-Universität,
D-4630 Bochum, Federal Republic of Germany

Long-slit measurements of angular correlation of annihilation radiation
(1D ACAR) have been performed with polarized positrons on six magnetized single
crystal specimens of the fcc ferromagnetic alloy $Co_{0.92}Fe_{0.08}$. The exchange
splitting between majority and minority spin electrons leads to a magnetic dif-
ference effect that varies between -1% at small angles and +6% at large angles.
Directional difference curves between differently oriented samples show aniso-
tropies up to 10%.

Calculations of the band structure with the average t-matrix approximation
(ATA) for several crystal potentials result in a single set of relatively sharp
d-bands (broadening less than 1-2 mRyd) with no sign of impurity levels. We
have therefore calculated the energy bands, the density of states and the momen-
tum density in the virtual crystal approximation. The results of these calcula-
tions for two non-selfconsistent crystal potentials are compared with angle-
resolved photoemission measurements with He, Ne and Ar UV-light on three samples.
This establishes the position of the majority spin X_2, X_5 levels at about
0.02 Ryd below the Fermi energy.

1D ACAR profiles have also been calculated. Directional difference curves
for Cu agree very well with measurements. For $Co_{0.92}Fe_{0.08}$ the calculations re-
produce the measured structure but the agreement is less perfect than for Cu
both at small and at large angles. The fit to the magnetic difference curves is
excellent at large angles but at small angles there are systematic discrepancies
that are little affected by considerable variations in enhancement. It is not
possible to indicate a preference for one of the two potentials.

From our results we draw the following conclusions:
1. The Fermi surface is rather well reproduced by either of the potentials used.
2. Wave functions calculated from the potentials used are not accurate enough
   to warrant detailed conclusions about enhancement corrections or the core
   contribution.

POSITRON ANIHILATION IN TRANSITION METAL CHALCOGENIDES (MX_2,MX_3)

T. Hatano, A. Suzuki, K. Ohtake, R. Yamamoto, M. Doyama
K. Endo*, H. Ihara*, K. Kaneko* and S. Gonda*
Department of Metallurgy and Materials Science, Faculty of Engineering,
The University of Tokyo, 7-3-1 Hongo Bunkyo-ku Tokyo 113, Japan
*Electrotechnical Laboratory, 1-1-4 Umezono Sakura-mura Niihari-gun,
Ibaragi 305, Japan

Transition metal chalcogenides have much interest in their non-linear conductivities, charge density waves, super conductings and probabilities of the solitary waves. Such remarkable phenomena with conduction electrons are due to the low dimensionalities of the Fermi surfaces and these low dimensionalities are results of the layered structures of the crystals. $MX_{2,3}$ have probabilities of changing their shapes of the Fermi surfaces and the densities of states at Fermi surfaces by means of the intercalation of donor or acceptor atoms between their layers and of the control of non-stoichiometricities of their compositions. Non-stoichiometricities can be controlled by the crystal growth conditions such as temperature and its gradient, pressure of chalcogen gases, diameter and length of the reaction tubes. Thus we can design their electron densities of states and their electron transport properties artificially and it is quite important to measure the electron density of states for further designing of the materials. Due to the imperfection of the crystals and the metal-insulator transition in low temperatures, other techniques can not be applied, and positron annihilation technique has a possibility to measure the electron density of states.

First we measure the positron lifetimes of $MX_{2,3}$, in order to distinguish the annihilation charactors of positrons in the layered crystals. A lot of small single crystals are stacked and wrapped with mylar sheets. And they are measured at room temperature with ^{22}Na source which is wrapped also mylar sheets thickness of 4µm. The source comporments were about 20%. In the case of $TaSe_3$ only one comporment of lifetime was found except of the source comporments (250psec). We conclude that positrons are insensitive for lattice defects which are highly concentrated non-stoichiometric vacancies and interstitials. At room temperature we can measure the electron densities of states by means of positron annihilation technique.

By the Doppler broadening measurement, anisotropic densities of states are obtained and the spectra shows s-like states of electrons. The Gaussian components are mainly come from the mylar sheets. The spectra are parabolic around the peak of the spectra and linear at the skirts on both sides, it is due to the low dimensionalities of the Fermi surfaces of the $MX_{2,3}$. (Fig. 1)
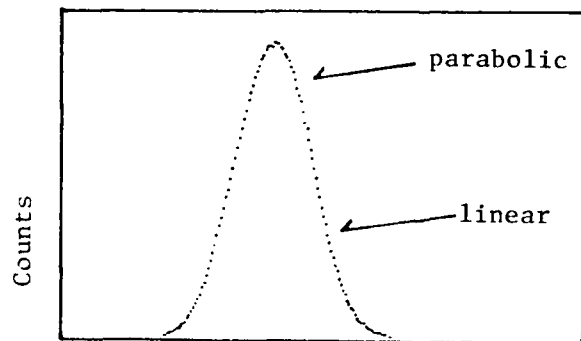
Channels
Doppler Broadening of $TaSe_3$
Fig. 1

RELATIVISTIC THEORY OF POSITRON ANNIHILATION IN SOLIDS OF HIGH ATOMIC NUMBER*

V. Devanathan and K. Iyakutti
Department of Nuclear Physics, University of Madras,
A.C.College Campus, Madras 600 025, India.

It is well known that for solids of high atomic number (Z), one has to use relativistic methods such as RAPW, RKKR and ROPW to compute the electron wave function. It has been shown[1], on the other hand, that non-relativistic methods are quite sufficient to obtain positron wave function in solids of high Z since positrons experience a repulsive potential and consequently their velocities do not increase with Z.

The two-photon annihilation probability is given by

$$F(\vec{p},\vec{k}) = \sum_{\text{spins}} |\Lambda(\vec{p},\vec{k})|^2$$

where $\vec{p}$ denotes the total momentum of the two annihilation photons and $\vec{k}$, the wave vector of the electron. Using the RAPW method to compute the electron wave function, the amplitude $\Lambda(\vec{p},\vec{k})$ can be conveniently written as a sum of two contributions f_i and f_o, one from inside the APW sphere and the other from outside since the wave functions assume different forms in these two regions. The contribution from outside the spheres is found by extending the form of the wave function in this region throughout the entire crystal f_o (crystal) and subtracting the resulting contributions from the regions inside the spheres f_o (spheres). Thus

$$\Lambda(\vec{p},\vec{k}) = f_i + f_o \text{ (crystal) } - f_o \text{ (spheres) }.$$

The terms f_o (crystal) and f_o (spheres) are identical with the corresponding non-relativistic terms[2,3]. The term f_i alone involves the actual relativistic wave functions for electron and positron. An exact expression has been derived for f_i which is shown to reduce to Louck's expression in the non-relativistic limit. The small component of positron wave function is always negligibly small and this, in turn, suppresses the positron annihilation probability arising from the small component of the electron wave function, which is no longer negligible in solids of high atomic number

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EMPIRICAL EQUATIONS FOR THE STOPPING POWER AND csda RANGE DIFFERENCE OF POSITRONS

D.K. Gupta, S.K. Gupta and J.C. Govil[&]
Physics Department, S.V. College, Aligarh
(Agra University) India

Empirical equations have been derived for the total stopping power and csda range difference of positrons in the energy region 0.2 to 10 MeV. These equations are valid for absorbers of atomic numbers from 1 to 92. Values of stopping power and csda range difference in elemental materials, compounds, detector materials and minerals obtained by using the present equations have proved to agree with reported values within a discrepancy of 3-4%.

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[*]Physics Department, D.S. College, Aligarh (Agra University)India.

ON UNDERSTANDING THE POSITRONIUM FRACTION IN LOW DENSITY PURE NOBLE GASES

R. E. Svetic and D. M. Schrader
Chemistry Department
Marquette University
Milwaukee, WI 53233, U.S.A.

Recent relative measurements of the positronium formation cross sections below the ionization potentials in low pressure helium and argon[1] permit quantitative estimates of the positronium fraction under the following assumptions: that the elastic scattering cross sections are smooth functions of positron incident energy, and that the distributions of the positron touch down energy (the energy of the first appearance of the positron in the region of interest) are constants.[2] These calculations give positronium fractions for helium and argon which agree exactly with the observations.[3]

Plots of the relative cross sections $\sigma_{Ps} / (\sigma_{Ps} + \sigma_{exc})$ between the excitation threshold and the ionization potential are practically identical for helium and argon, and can hence be used also for the other noble gases. Calculations again agree exactly with experiment for neon, but for krypton and xenon the calculated fractions (0.38 and 0.44, resp.) are much higher than observed values (0.16 and 0.03[4]). Even the lower Ore estimates (0.20 and 0.26) are too high.

To resolve this dilemma, the two assumptions above are tested by subjecting them to critical calculations. That is, the elastic cross sections in the positronium region are re-calculated using an improved version of a successful semiempirical quantum mechanical method[5], and the touch down distributions are calculated from the data of Coleman, et. al[6]. The effect of van der Waals associates is also considered.

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POSITRONIUM FORMATION IN DENSE GASES

Finn M. Jacobsen

Chemistry Department, University of Alberta, Edmonton, Alberta, Canada T6G 2G2
Permanent Address: Chemistry Department, Risø National Laboratory, DK-4000
Roskilde, Denmark

In recent years the positronium (Ps) fraction has been measured in a quite large number of atomic/molecular dense gases and in mixtures of densed gases. In a number of cases the Ps fraction has been found to depend on density, temperature and composition (mixtures) in an unexpected way. Two different models of the Ps formation processes are in use at present. In very low density gases the Ore model[1] is used to interpret the measured results while in high density liquids the spur model[2] is applied. At these density limits both models are well accepted today. In the present talk we shall discuss the possible influence of the behaviour of secondary/excess electrons on the Ps yield in dense gases as function of temperature, density and composition (mixtures). After a short introduction to the experimental work on the properties of secondary/excess electrons in gases we will discuss phenomena such as: thermalization range of secondary electrons, excess electron mobility (state of thermalized excess electrons), secondary ionization events (in mixtures of gases), etc.

In most gases experiments have shown that electron spurs are formed at densities well below $0.1 \, n_c$, where n_c is the critical density, however in the atomic gases He, Ne, and Ar no experimental results support electron spur formation even at densities as high as n_c. The latter is perhaps in agreement with the density independence of the Ps fraction in these gases.

Finally we will suggest some future experiments to be performed in order to further investigate the influence of the behaviour of secondary/excess electrons on the Ps fraction.

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POSITRON-ION COLLISIONS:
POSITRONIUM FORMATION FROM HYDROGENIC IONS

Sunanda Guha[*] , Chandana Sinha and N.C.Sil
Department of Theoretical Physics, Indian Association for the
Cultivation of Science, Calcutta 700032, India

*Dept of Physics, Lady Brabourne College, Calcutta 700017, India

The positronium (Ps) formation as a result of electron capture by positrons from hydrogenic ions such as He^+ and Li^{2+} has been investigated using the Coulomb Born (CB) approximation where the long-range Coulomb interaction between the incident positron and the target ion has been accounted for. We have also attempted to make an improvement[1] over the CB approximation by retaining in the two-state coupled equations, the first-order term that was neglected in the CB approximation. By virtue of such consideration one can get rid of the defect inherent in the CB approximation for charge transfer problems arising from the lack of orthogonality between the initial and the final states. This approximation is to be called the Modified Coulomb Born approximation (MCB). Differential and total cross sections for the Ps formation have been computed in the CB and MCB approximations for different isoelectronic ions at several incident energies. Since the wave functions of hydrogenic ions are exact there is no question of any post-prior discrepancy. From these results it is found that the MCB capture cross section gets considerably reduced in the low-energy region while at high energies the MCB results are higher than the corresponding CB results. The CB results monotonically increase with decreasing energy whereas the MCB results exhibit a peak at different intermediate energies for different target ions. The differential cross section in the CB approximation falls sharply from a forward peak, becomes zero at an angle depending on the projectile energy and then rises again to a maximum to fall monotonically afterwards with the increase of the scattering angle. In MCB on the other hand, the differential cross section above 100 eV (in case of He^+) does not show up any such behaviour but below 200 eV its feature is more or less the same as that of CB. Some preliminary results have been presented in table I.

TABLE I.   Capture cross sections in units πa_0^2

| Energy in eV | Hydrogenic Ions | | | |
| | He^+ | | Li^{2+} | |
	CB	MCB	CB	MCB
75	5.309(-2)	3.937(-2)		
100	4.518(-2)	3.989(-2)		
200	9.982(-3)	1.060(-2)	4.040(-3)	3.121(-3)
500	3.113(-4)	3.912(-4)	5.707(-4)	6.037(-4)

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POSITRON-ION COLLISIONS:
POSITRONIUM FORMATION FROM HELIUM-LIKE IONS

A.C.Sil, Chandana Sinha and Sunanda Guha*
Department of Theoretical Physics, Indian Association for the
Cultivation of Science, Calcutta 700032, India

*Dept of Physics, Lady Brabourne College, Calcutta 700017, India

The Coulomb Born (CB) approximation and a modified version of
it (MCB) where distortion has been taken into account in the ini-
tial channel have been applied to calculate the positronium (Ps)
formation cross sections under the impact of positrons with
helium-like ions. The ground state wave functions of the helium-
like isoelectronic series and the corresponding experimental ener-
gies have been taken from Morse et al.[1]
Some preliminary results for the processes

$$e^+ + Li^+(1s) \rightarrow (e^+e^-) + Li^{2+}(1s)$$

$$e^+ + Be^{2+}(1s) \rightarrow (e^+e^-) + Be^{3+}(1s)$$
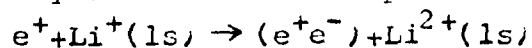
are presented here taking account of the full interaction. The CB
results in the post and prior forms are found to agree within 15%
throughout the energy range considered. In the case of the MCB
approximation the initial and final channels are not treated on
equal footing, the former being given a special bias and the prior
form interaction appears naturally.

As may be noted from table 1, the total cross section increa-
ses monotonically with decreasing energy. The effect of the present
modification over the CB approximation is to reduce the capture
cross section in the low energy region significantly while at high
energies (e.g. 500 eV for Li+) the MCB cross sections are higher
than the CB ones. We have also studied the differential cross sec-
tion for the CB (post and prior) as well as the MCB approximation.
The CB differential cross section falls sharply from a forward peak
to reach a minimum and then rises upto a second broad maximum to
fall again smoothly with the increase of the scattering angle. The
MCB differential cross section on the other hand, becomes zero at
some scattering angle below a specific energy (viz 500 eV for Li+)
and beyond that energy it does not show up any such behaviour.

TABLE 1.   Capture cross sections in units of πa_0^2

Energy in eV	Ions					
	Li+			Be²⁺		
	CB		MCB	CB		MCB
	Prior	Post		Prior	Post	
100	4.483(-2)	4.696(-2)	1.333(-2)			
200	1.741(-2)	1.924(-2)	1.182(-2)	5.250(-3)	5.083(-3)	1.573(-3)
500	1.075(-3)	1.020(-3)	1.126(-3)	1.187(-3)	1.262(-3)	9.216(-4)
1000	5.581(-5)	5.122(-5)	7.372(-5)	1.127(-4)	1.093(-4)	1.173(-4)

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POSITRONIUM FORMATION IN POSITRON-HYDROGEN SCATTERING

Priti Khan
Muralidhar Girls' School, Calcutta 700029, India

A.S. Ghosh
Department of Theoretical Physics
Indian Association for the Cultivation of Science
Jadavpur, Calcutta 700032, India

The formation of positronium atom in its ground state in positron-hydrogen scattering is considered here. s-wave cross sections has been obtained variationally by Chan and Fraser,[1] Stein and Sternlitsch[2] and Hamberston[3] and p-wave by Chan and McEachran[4] . Drachman et al[5] have taken the results of Canadian group for $\ell=0$ and 1 and replaced the contributions of higher partial waves by first Born approximation. Their results are in good agreement results of Winick and Reinhardt[6] . It is well known that Born results are not suitable for rearrangement channel. We have investigated the problem in which total wave function is represented by polarized orbital one. The matrix element is given by

$$T_{if} = \left\langle \omega_{1s}^*(r_{12}) X(s) \left(\frac{1}{r_1} - \frac{1}{r_2}\right) \left\{ \Phi_{1s}(r_2) + \Phi_{pol}(r_1,r_2) \right\} F(r_1) \right\rangle \tag{1}$$

where $\omega_{1s}^*(r_{12})$ and $X(s)$ represent positronium atom in its ground state and moving positronium respectively. Here $\Phi_{1s}(r_2)$ and $\Phi_{pol}(r_1,r_2)$ are the undistorted and distorted wave functions of atoms respectively. $F(r_1)$ satisfies the following differential equation

$$\left(-\frac{1}{2}\nabla_{r_1}^2 - k_{1s}^2 + V_s - V_p \right) F(r_1) = 0 \tag{2}$$

where V_s and V_p are the static and polarization potential s respectively.

Two different sets of results for total Ps-formation cross sections have been primarily obtained. First set contains the s- and p-wave results of variational calculation with higher partial waves results obtained by using relation (1). Second set is the results of relation (1) for all partial waves. The results will be presented at the Conference.

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POSITRONIUM FORMATION IN POSITRON-HYDROGEN COLLISIONS

G. Banerji[*], P. Mandal[+] and A. S. Ghosh[+]

[*]Burdwan University, Burdwan 713 104, India

[+]Indian Association for the Cultivation of Science,
Calcutta 700 032, India

The positronium formation problem in positron-hydrogen collision has been investigated by different workers[1]. The results obtained so far for this rearrangement collision process are not satisfactory[1]. Reliable results for the positron-hydrogen elastic scattering have been obtained by Banerji et al[2] using a polarized orbital method. This form of polarized orbital method includes the adiabatic and non-adiabatic potentials in both the direct and the rearrangement channels. Here this method is used to study the positronium formation in the ground state from atomic hydrogen by positron impact.

The coupled integral equations have been given by Datta et al[3] who have obtained the elastic cross sections above the positronium-formation threshold. These equations are solved numerically and the cross sections for positronium formation are obtained as usual. In Fig 1 we display the differential cross sections for incident positron energy 10.2 eV. The present results are compared with the corresponding results of other calculations.[4]
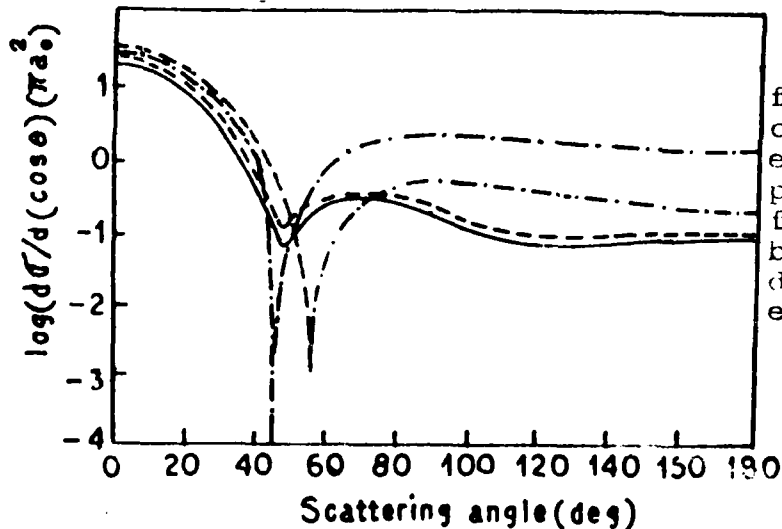
Fig 1. Positronium formation differential cross sections for positron energy 10.2 eV. Solid line: present work; dotted line: first Born approximation; broken line: Basu et al; double dotted line: Mandal et al.

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OBSERVATION OF THE 1^3S_1-2^3S_1 ENERGY SPLITTING IN POSITRONIUM

A. P. Mills, Jr. and S. Chu

Bell Laboratories, 600 Mountain Avenue, Murray Hill, NJ   07974 USA

We report the first observation of the optical excitation of Ps and show that high precision optical measurements of the Ps energy level structure are now possible. Our measurements are made possible by (i) the development of high intensity,[1] pulsed[2] slow positron sources; (ii) the discovery of thermal energy positronium emission from metal surfaces[3]; (iii) the development of high-power narrow-band tunable laser sources; (iv) the use of two photon Doppler-free techniques that allow the entire Doppler distribution of atoms to be excited simultaneously[4]; and (v) the use of single atom detection techniques.[5]

The Ps source consists of a slow positron beam feeding a magnetic +rf storage bottle, a time-bunching accelerator, and a Cu(111) + S e^+ target which forms the thermal Ps atoms. Using a $\sim$ 200 mCi ^{58}Co source, about 25 e^+'s hit the target in 8n sec FWHM pulses. Under our experimental conditions, $\sim$ 6 of these positrons are quickly re-emitted as slow positrons, $\sim$ 4 are desorbed from the surface as thermal 1^3S_1 Ps, and the remainder either annihilate ($\tau < 1$ nsec) or escape as non-thermal ($\sim$ 3 ev) Ps.

A narrow-band, Yag-pumped dye laser (Littman-Metcalf oscillator[6] plus inter-cavity etalon, 18 mj/pulse, $\sim$ 10 nsec pulse width, 10 pulse per sec) is used first to excite the 2 photon-allowed[7] $1^3S_1 \rightarrow 2^3S_1$ transition and then to photo-ionize the Ps atom from the 2^3S_1 state. The e^+ ionization fragment is collected with $\sim$ 50% efficiency, directed through an ExB velocity filter that rejects stray ions, and finally detected by a 2-stage microchannel-plate detector. We discriminate with > 99% efficiency the copious slow e^+ re-emitted from the Cu target ($\sim$ 2 counts/pulse) from the ionized 2^3S_1 Ps ($\sim$ 0.03 counts/pulse on resonance) by delaying the light pulse 30 nsec with respect to the e^+ pulse.

The result of our first successful ½hr. scan in the vicinity of the 1^3S_1-2^3S_1 resonance shows a resonance peak about 2 GHz wide and about 13 σ's above the background level. A frequency marker, calibrated on the H-D Balmer-β transitions, is used to measure the laser frequency shift relative to the D$_\beta$ transitions. The resonance occurs 120 ± 2 GHz to the blue of the D$_\beta$ calibration and is consistent with the α^2Ry calculations of Ferrell.[8] The line-width is primarily due to the high ionization rate, the laser band-width, and the DC Stark-shift in an inhomogenous electric field. The precision of this measurement is already at the level where the α^3Ry terms are needed (the first-level loop diagrams). These terms have been calculated for the n=2 state by Fulton and Martin[9] and can be modified for the n=1 state.

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EVIDENCE OF EXCITED STATE Ps FORMATION
FROM A CLEAN METAL SURFACE IN ULTRA-HIGH VACUUM*

D. Schoepf, S. Berko, K. Canter, A. Weiss
Physics Department, Brandeis University
Waltham, Massachusetts 02254, U.S.A.

We report on the first observations of excited state positronium formation from a clean metal surface in ultra-high vacuum. Our preliminary experiments obtained using a Cu[100] sample show a formation efficiency of about one excited state per 10^3 incident slow positrons. This is to be compared to previous results[1,2] of between one in 10^4 and one in 10^3 obtained from uncharacterized surfaces in a 10^{-7} to 10^{-8} torr vacuum.

Slow positrons are obtained from a Cu[111] converter in a backscattering geometry[3] and electrostatically guided and focussed[4] at 200 eV onto a target of Cu[100] crystal which is maintained at a retarding potential to yield incident positron energies in the range 0 to 20 eV. The Cu target is viewed by a UV-sensitive photomultiplier through a Suprasil-quartz window to detect 2P→1S Lyman-α optical transitions. Diametrically opposite to the UV photomultiplier is a 3"×3" plastic scintillator to observe the annihilation γ-rays from ground state positronium decay. Decay events of the form $2^3P \rightarrow 1^3S \rightarrow 3\gamma$ are detected by a delayed coincidence measurement of a Lyman-α photon ($2^3P \rightarrow 1^3S$) followed by an annihilation γ-ray ($1^3S \rightarrow 3\gamma$). The resultant delayed coincidence spectrum contains the long lifetime component of 1^3S positronium as a signature of excited state formation. Observation of the counting rates in the long lifetime component region of the delayed coincidence spectrum serve as our monitor of excited state production. Experiments involving 2^3S production will be performed in the future by adding an r-f field to induce $2^3S \rightarrow 2^3P$ transitions and observing the relative increase in this delayed region.

Counting rates in the delayed region were taken at several incident positron energies between 0 and 20 eV and show a statistically significant threshold near 2 eV. Using the delayed spectrum obtained for incident positron energies less than this threshold as an "off" spectrum and subtracting this from the spectrum for incident positron energies greater than threshold, we obtain a spectrum which has a long lifetime component statistically consistent with the 140 nsec lifetime of 1^3S positronium.

Experiments in progress hope to determine the excited state production from other metallic surfaces, such as W and Cr, which have large negative positron work functions and are hence good candidates for n=2 Ps formation. Future experiments will also characterize the excited state production as a function of temperature, incident positron energy and metal surface contamination.

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EXACT FIRST ORDER ELECTRON SELF-ENERGY CONTRIBUTION
TO THE DECAY RATE OF ORTHOPOSITRONIUM

Michael A. Stroscio
Air Force Office of Scientific Research
Directorate of Physical and Geophysical Sciences
Bolling Air Force Base
Washington, DC 20332
USA

The exact electron self-energy contribution to the decay rate of orthopositronium to order α^7 is formulated and explicitly derived. This Feynman gauge result provides a stringent check on previous numerical calculations and serves as a benchmark for future computations based on symbol manipulating algorithms.

The lowest order, nonradiative decay rate is,[1]

$$\Gamma_a = \frac{2}{9\pi} \frac{\alpha^6 mc^2}{\hbar} (\pi^2 - 9).$$ (1)

The exact matrix element and the decay rate for the electron self-energy contribution were formulated in the Feynman gauge and are given by,

$$\Gamma_{bc} = \frac{\alpha^7 mc^2}{\pi^2 \hbar} \left[\frac{-7}{6} + \frac{805}{1296} \pi^2 + \frac{67}{18} \ln 2 - \frac{775}{1944} \pi^2 \ln 2 - \frac{1049}{324} \, (3) \right]$$

$$+ \frac{\alpha^7 mc^2}{\pi^2 \hbar} \left[\frac{8}{9} (\pi^2 - 9) \ln(\lambda/m) \right].$$ (2)

Previous numerical approximations [2,3] to Eq. (2) have been expressed in terms of the ratio, Γ_{bc}/Γ_a. From Eqs. (1) and (2),

$$\frac{\Gamma_{bc}}{\Gamma_a} = (4.78498 + 4\ln(\lambda/m))(\alpha/\pi).$$ (3)

This value agrees with the numerical results of Stroscio and Holt.[2] On the other hand, the numerical integration of Caswell et al.[3] resulted in the numerical coefficient 4.791 ± 0.003. Both the exact and the precise numerical values of the present work disagree with the result of Ref. 3.

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DO e^+-LIFETIMES REFLECT THE AGE OF THE UNIVERSE?

J.T. Muheim
Laboratory of Solid State Physics, Swiss
Federal Institute of Technology, Hönggerberg,
CH-8093 Zürich (Switzerland)

According to the model of cosmological parameters derived from the spot conditions of the spark mass plasma and applied to the gravitational situation of the expanding universe (1), the Hubble constant is a structural quantity which may be expressed in physical constants and has the constant value $H_g = 16,08$ km s^{-1} MLy^{-1} ($= 1,700.10^{-18}$ s^{-1}). On the other hand the Hubble Law, $v = H_g R$ is valid only in the scale range $2,3.10^7 \lessgtr R \lessgtr 10^{10}$ Ly. In view of this model, which presupposes only 5 constants, i.e. $e_s, \hbar, c, G$ and k_B, $\tau_g = 1/H_g$ stands for a time equivalent to a relaxation time of the gravitational interaction and has no relation to the actual age of the cosmos. As demonstrated recently (2) there exists a formal equivalence between the gravitational recession of the universe since the Big Bang and the spark-induced weak interaction recession of the exploding solid. Furthermore, since the optical Lyman spectrum of hydrogen corresponds to the space-time structure of the cosmos, the Rydberg constant and the hyperfine frequency are related in a simple way to the Hubble constant.

Therefore, if it is not the Hubble recession, which physical processes are then related to the age of the universe? One possible answer is: certain lifetimes. Consider the e^+-lifetime which can be measured in the laboratory. Even in an ideally perfect insulating solid of infinite extent the e^+-lifetime is finite as a result of the perturbing action of the background photons. If we succeed in correcting for the influence of the chemical bond we may obtain a lower limit for the radiation-induced lifetime. This has been done by using the τ-data of the Milano group (3) and by extrapolating to a zero influence of the chemical bond ($\Delta x_{MX} \to 0$). Owing to the empirically ascertained quasiequivalence of MX interaction rates (4), we may assume the weak interaction to be equally responsible for e^+-annihilation in the same way as for the plasma recession. In this way and by taking into account the régime of flux quantization, we obtain, on the basis of either the average bondfree "covalent" or "ionic" lifetimes, a lower limit for the universal age of $(13,2\mp1,5).10^9$ y respectively $(14,2\mp1,5).10^9$ y. The corresponding upper limit for the temperature of the relic radiation amounts to 4,0 K and 3,7 K respectively, in excellent agreement with observation.

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A MODEL FOR THE SHELF
IN THE DIFFUSE γ-RAY SPECTRUM

Richard L. Liboff
Schools of Applied Physics and Electrical Engineering
Cornell University, Ithaca, N.Y.   14853
and
Daniel M. Heffernan
Dublin Institute for Advanced Study, Dublin 4, Ireland

A model is proposed to describe the observed shelf in the cosmic diffuse radiation spectrum just above 1MeV. This model is based on induced positronium annihilation in which a photon of frequency ω and wavelength λ interacts with a positronium atom at rest and annihilates it to yield two photons of frequency ω_1 and ω_2. These photons emerge at angles θ_1 and θ_2, respectively, with respect to the incident photon direction. Taking the positronium atom to be a particle of mass 2m (m is electron mass), a simple Compton-like calculation yields the following relation for the wavelength λ_1.

$$\lambda_1 - \lambda = \lambda_C \left[\sin^2 \frac{\theta_1}{2} - \frac{\lambda_1 \lambda}{\lambda_C^2} \right]$$

Here $\lambda_C = h/mc$, is the Compton wavelength. Conservation equations further yield that $\omega_1 = \omega_2 = \omega$ whenever $\omega_1 = 2\omega_C$, ($\lambda_1 = \lambda_C/2$), corresponding to incident photon energy, $2\hbar\omega_C^2 = 2mc^2 \simeq$ 1MeV, and an angular separation 60° of the two emergent equal-frequency photons. These photons in turn can induce two other positronium atoms to annihilate to yield two photons of frequency $2\omega_C$ traveling parallel to the original incident photon. Thus, after two path lengths, an incident photon flux of frequency $2\omega_C$ will be doubled. Hence, for a continually regenerated electron-positron plasma whose extension is greater than the mean free path of the $2\omega_C$ photon in the plasma, an incident flux of 1MeV photons will be amplified by this process. It is proposed that this amplification may occur in double radio sources or other cosmic accreting objects.

SINGLE-POSITRON ANALYSIS FOR THE STUDY
OF TRANSIENT ELECTRONIC PROCESSES IN INSULATORS*

L.Yarmus, V.P. Shantarovich[+], and Werner Brandt
Radiation and Solid State Laboratory
New York University, New York, New York 10003, USA

Energetic positrons injected into a medium from a radioactive source cause electron-ion pair formation. Our object is the study of elementary transient processes leading to electron-ion recombination as a function of the physical parameters of the medium. To this end, consider an insulator with a small concentration of fluorescent centers as markers. On electron-geminate ion recombination of a marker, the fluorescence light is registered in a single-photon detector in coincidence with the birth signal of the positron.

The experiment proceeds in two steps. First, it registers the delayed fluorescent lifetime distribution. It is indicative of the recombination time spectrum of the electron-ion pairs.[1] This spectrum is characteristic of the medium in which the markers are dispersed. Second, transient-electron states in the medium cannot be studied by conventional electron paramagnetic resonance (EPR) techniques because of the short lifetimes of the electron-ion pairs. But EPR of transient states can be studied optically,[2] because they manifest themselves through resonance structures in the intensity distribution of the recorded delayed fluorescent lifetime spectra. Such resonance structures moreover may depend on the time delay.

An instrument is under construction in which sample and ^{22}Na source are placed inside a resonant cavity and coupled to two photomultipliers (PM) through light pipes. One PM monitors the 1.3MeV gamma ray emitted with a positron from the source. The other PM, through slits, responds to a single fluorescence photon from a marker in delayed coincidence with the 1.3-MeV gamma ray. Our first project is to measure subexcitation electronic stopping powers[3] in organic liquids.

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POSITRON ANNIHILATION IN HETEROGENEOUS SUBSTANCES

V.P. Shantarovich, L.G. Aravin, V.A. Onischuk, B.M. Levin and
V.I. Goldanskii
Institute of Chemical Physics Academy of Sciences of the
USSR, 117334 Moscow, Vorobjevskoe Shausse 2b, USSR

Consider substances composed of two different materials dispersed to dimensions D comparable to or smaller than the positron diffusion length Λ until annihilation, i.e., $\Lambda \gtrsim D$. Positron annihilation characteristics are influenced by the properties of the materials as well as by positron diffusion to or through interfaces.[1]

Application of the Brandt[2] model to the data reduction leads to the separation of annihilation components from the two materials and the interface. This permits inferences about grain surface properties and the chemical interaction between grains and matrix. We found the positron method useful in structural studies of a number of heterogeneous systems. (1) In aerosil-filled vulkanized rubbers, polymer molecules are attached to filler surfaces, which is important for the reinforcement of the material.[3] Epoxi resins were found to lack uniformity in crosslinking. Differences of kinetics of poly-4-methyl-pentene oxidation in the crystaline and amorphous states could be distinguished.[4] The interpretation is based on the annihilation characteristics of positronium in the free volume.[5] (2) Positronium formation in insulators, near highly dispersed Pd grains was found to be grain-size dependent,[6] which can be related to the size-dependent metal work function.[7] (3) Micellae in water solutions show strong variations in annihilation characteristics due to positron trapping by micellae.[8,9] (4) The positron lifetime method was also used in studies of the incipient stages of new-phase formation in Si glasses,[10] shock-wave treated iron oxides, and aged martensitic steels.

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POSITRON ENERGY LOSS MEASUREMENTS IN THIN SINGLE-CRYSTAL SILICON AND POLYCRYSTALLINE CARBON FOILS

K. G. Lynn, W. Frieze* and D. Fischer
Brookhaven National Laboratory**
Physics Department
Upton, New York 11973, U.S.A.

Energy loss measurements were performed with a controllable energy (0.1 - 7.0 keV) electrostatically focussed positron beam on a thin single crystal Si sample (∼2000 Å thick) and a polycrystalline carbon foil (∼500 Å). The transmitted positrons were energy analyzed using a high transmission four-grid retarding field analyzer coupled with a two-stage channel electron multiplier plate with a phosphorus screen as a final stage. Results for the elastic and inelastically scattered positrons will be presented for both samples.

STUDY OF VACANCY-SOLUTE INTERACTIONS IN DILUTE LEAD BASED ALLOYS
BY THERMAL EQUILIBRIUM MEASUREMENTS OF ANNIHILATION LINESHAPES

K. Ito, Y. Ohtsu and S. Tanigawa
Institute of Materials Science, University of Tsukuba,
Sakura-mura, Ibaraki 305, Japan

It is well established that self-diffusion in most metals occurs predominantly by a vacancy mechanism. On the other hand, it is well known that some solute atoms in lead show very fast diffusion. In the present paper, the thermal equilibrium measurements of Doppler broadening of annihilation radiations were applied to a series of dilute lead based alloys. Experiments were carried out on 99.9999% pure lead, Pb-0.01at.%Au, Pb-0.015at.%Ag, Pb-0.3at.%Cu, Pb-0.3at.%cd and Pb-0.5at.%Sn. The summary of the results is shown in Fig. 1. Experimental features in lead based dilute alloys are quite different from those in aluminum based dilute alloys which will be presented as a separate paper at the conference. The threshold temperature in each lead based alloy for the onset of vacancy effect seems to remain little changed from that in pure lead. The only one difference from pure lead is that the fraction of variation in lineshape parameters from 25°C to 300°C is lower than pure lead. This trend becomes stronger as increasing the valency of solute elements. If we define the fractional ratio of change in S parameter as $\eta = [S(300°C)-S(25°C)]/S(25°C)$, it was found that $\eta(Pb) > \eta(Pb-Cu) \simeq \eta(Pb-Au) \simeq \eta(Pb-Ag) > \eta(Pb-Cd) > \eta(Pb-Sn)$ in accordance with the valency of solute elements. The suppression of vacancy effect can be considered in the following two ways. In the first, this fact may be caused by the existence of repulsive interactions between a vacancy and a solute atom in these alloys. That is, the available sites for the formation of single vacancies may be reduced by the addition of solute atoms with repulsive interaction. In this case, interactions may extend over a several atomic distances. In the second, this fact may be corresponding to the formation of vacancy-solute pairs and may be caused by the decrease in the trapping rate of positrons. If a solute atom substitutes with lead atom adjacent to a vacancy in a simple way, it can not be understood that the fractional ratio in every alloy is lower than in pure lead. Therefore, the configuration of vacancy-solute pairs may be considered as follows: A solute atom occupies an interstitial site near a vacancy. If so, the decrease of trapping rate can be well interpreted. Furthermore, the valency effect can be well interpreted. However, in the present stage, above two alternative ideas are only speculative.
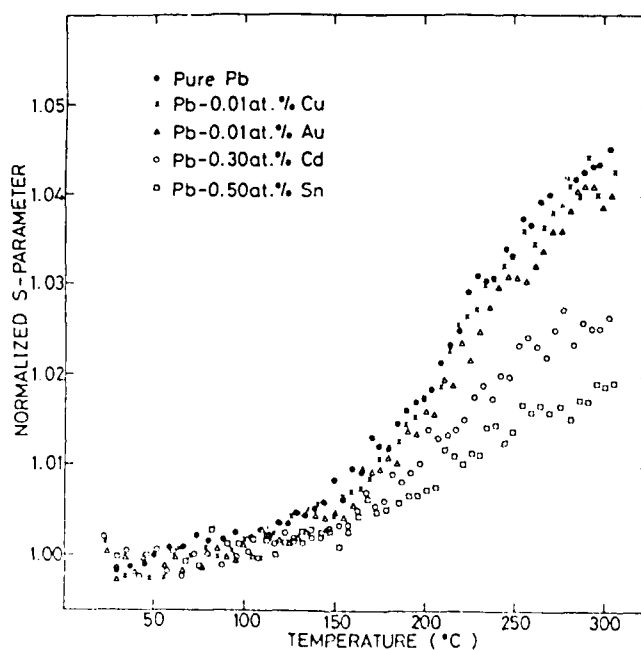
Fig. 1

INVESTIGATION OF HELIUM IRRADIATED STAINLESS STEEL BY POSITRON ANNIHILATION

B. Viswanathan[+], G. Kögel and W. Triftshäuser
Hochschule der Bundeswehr München, D-8014 Neubiberg, Germany

Austenitic stainless steel 316 is a single phase alloy with the same fcc structure as nickel and is a leading candidate material for fuel cladding of fast breeder reactors and for first wall of fusion reactors. Therefore helium-vacancy properties are of particular importance in this material. Here positron annihilation measurements are reported in α-irradiated SS 316. 500 μm thick specimens were solution treated at 1200°C and cooled in argon atmosphere to produce a controlled state for irradiation (measured lifetime of this state is 115 ps). Uniform implantation of helium was made at ambient temperature to a depth of 100 μm from the surface, using a cyclotron beam of 28 MeV α-particles as well as an energy degrader in the beam path. The implanted helium dose was 500 at.ppm. Positron measurements were started several weeks after irradiation, using Doppler broadening and precision timing systems for simultaneous measurements of lineshape and lifetime. The defect evolution was traced during post-irradiation isochronal annealing stages in close steps.

Analysis of lifetime and Doppler lineshape parameters reveals the following three main stages: (A) An early stage of defect recovery until 450°C essentially indicates the thermal dissolution of vacancy loops, located in the damaged region. (B) A stage between 450°C and 700°C where the Doppler lineshape parameter I_v starts to increase again. This indicates additional positron trapping. The lifetime component τ_2 increases steadily from 190 ps towards larger values. This is consistent with the defect-specific R-parameter behaviour. (C) A stage after 700°C. Here the I_v parameter starts decreasing having reached a maximum value at 700°C. The R-parameter tends to stabilise. No lifetime associated with dislocation loops is seen in this region. Two characteristic lifetime components ($\tau_2 \sim 330$ ps and $\tau_3 \sim 500$ ps) are detected with a satisfactory fit, in addition to the bulk component τ_1 . Even at 1200°C no recovery to the unirradiated state is observed in this helium implanted material. The consistency of the current positron results in the stage (C) with the reported TEM results on the same material is discussed. On the basis of the correlated behaviour of lifetime and lineshape parameters, interpretations are given for the mechanism of helium bubble nucleation and growth.

+ On leave from: Reactor Research Centre, Kalpakkam - 603102, India

DEFECT INTERACTIONS IN LEAD DILUTE ALLOYS

Y.Hara and S.Nanao

Institute of Industrial Science, University of Tokyo
7-22-1, Roppongi, Minato-ku, Tokyo 106, Japan

Silver and cadmium in lead are known as so-called fast diffusers, although they diffuse in lead rather slower than extremely fast diffusers such as nickel, paradium and copper. The atomic radius ratios of the solute to the solvent in the fast diffusion systems are out of ranges suitable for the formation of interstitial alloys and substitutional ones known as Hagg's rule and Hume-Rothery's rule, respectively. In these alloys, the solute atoms bring large strain to the lattice around them and are expected to gave intensive interactions with vacancies and/or their clusters. The interaction between the solute and the lattice defects in these alloys will change positron lifetime parameters.

In the present study, positron lifetimes in Pb, Pb-Ag and Pb-Cd were measured in equilibrium states. The specimens are Pb, Pb-0.015at% Ag, Pb-0.17at%Ag and Pb-0.2at%Cd prepared from 6N lead, 5N silver and 6N cadmium. They were chemically polished and annealed at 580K in a vacuum for 24 hours. The lifetimes were measured as a function of termperature from 300K to 580K in a vacuum below 10^{-3}Pa with the high rate lifetime analysis system. Each spectrum has total counts of 4 to 7 $\times 10^{6}$ and peak counts of 1 to 2 $\times 10^{5}$.

The spectra obtained below 380K were analysed with three components relating to the specimen and the source, one for the former and two for the latter. Above 380K, the number of fitting components were two for the specimen and the source components were fixed at the values which were determined from the spectra below 380K.

Tnere observed no appreciable differences between the parameters in Pb-Ag and those in pure Pb within the temperature range of below 500K. This suggests that the binding enthalpy between a mono-vacancy and a silver atom is below 0.1eV. The difference was detected at the temperatures above 500K. At these temperatures, the values of the mean lifetime in Pb-Ag were slightly larger than those in pure Pb, which probably indicates the strong interaction between di-vacancies and silver atoms.

From the values of the mean lifetimes in pure Pb, vacancy formation enthalpy Ev was tentatively evaluated to be 0.55eV with the least square method. The apparent value of Ev in the Pb-Ag alloy was estimated to be the same within experimental errors.

POSITRON ANNIHILATION MEASUREMENTS OF VACANCY FORMATION IN Ni and Ni(Ge)[*]

L. C. Smedskjaer, M. J. Fluss, D. G. Legnini, M. K. Chason, and R. W. Siegel
Materials Science Division, Argonne National Laboratory
Argonne, Illinois 60439, U.S.A.

Vacancy formation in Ni and in dilute Ni(Ge) alloys is being studied under thermal-equilibrium conditions using the positron annihilation Doppler-broadening technique. Measurements were performed initially on Ni samples of 99.995 wt.% purity, which had been annealed in an ultra-high vacuum (10^{-8}-10^{-9} Torr) chamber at $\sim 30°C$ below their melting point for $\geqslant 2$ h prior to the in situ measurements. A value of the monovacancy formation enthalpy, $H^F_{1v} = 1.8 \pm 0.1$ eV, was determined from these data. This result will be compared with previous positron annihilation and quenching results for Ni. In addition, a value for the monovacancy migration enthalpy in Ni, $H^M_{1v} = 1.1 \pm 0.1$ eV, was deduced from a comparison of the present H^F_{1v} measurement with previous self-diffusion results; this will be compared with the available vacancy-mobility information. Measurements on a 1 at.% Ni-Ge alloy sample indicate a high apparent vacancy-solute binding enthalpy (> 0.5 eV) and, therefore, subsequent Doppler-broadening measurements of vacancy formation in alloys with < 1 at.% Ge are now being performed. These results will be presented along with their interpretation in terms of vacancy-solute binding. Comparisons with theoretical predictions and the available experimental results regarding the effects of vacancy-solute binding in this alloy system will be made.

THE DEPENDENCE ON CRYSTAL ORIENTATION OF
ANNIHILATION LINESHAPES FOR LOCALIZED POSITRONS

M. Selen and I. K. MacKenzie
Department of Physics, University of Guelph
Guelph, Ontario, Canada
N1G 2W1

The width of the momentum distribution for annihilating
pairs is shown to depend strongly on both crystal orientation
and temperature for several anisotropic metals. Localization
in the prevacancy region produces highly anisotropic dis-
tributions whereas vacancy saturation results in a close
approach to spherical symmetry. Rotation patterns are also
given for vacancies and non-equilibrium defects in β brass.

VACANCY FORMATION ENERGIES IN ALLOYS

S.M. Kim

Atomic Energy of Canada Limited, Chalk River Nuclear Laboratories,
Chalk River, Ontario, K0J 1J0, Canada

Although vacancy formation in alloys has been studied experi-
mentally and theoretically for many years, a coherent picture has not
been available. Recently, however, we have found that there exists a
simple empirical relationship between the formation energies of al-
loys and those in the constituent pure metals for the bcc, fcc and
hcp structures. With this relationship it is possible to predict the
formation energies of vacancies in various alloys, and to determine
the vacancy formation energies of pure metals in these structures.

A new model of vacancy formation in ordered bcc AB type alloys
(CsCl structure) will be presented. In these alloys we find that the
vacancy formation energy is given by $E(AB)=E(B)+8v$, where $E(B)$ is the
vacancy formation energy of metal B in the bcc phase $(E(A) > E(B))$ and
v is the ordering energy. We also find that monovacancies form only
on the A atom sublattice. As the alloy disorders, however, the
distinction between the A atom and B atom sublattices disappears and
divacancies begin to form. These results are consistent with the
observed vacancy properties in the bcc AB type alloys.

Positron Annihilation Study of $Ni_{75}Cr_{15}Fe_{10}$ Alloy

Peng Yuqing, Zheng Wanhui, and Zhu Jiabi
Shanghai Institute of Nuclear Research, Academia Sinica
Wang Jingcheng
Shanghai Institute of Iron and Steel Research

The K-State and defects of $Ni_{75}Cr_{15}Fe_{10}$ alloy have been investigated using positron annihilation technology.

The temperature dependence of positron lifetime and lineshape parameter of annihilation radiation in region of 300°C-800°C were measured. The K-State of this alloy presented at about 500°C.

In order to estimate dislocation density and vacancy concentration of the plastic deformed samples, lineshape parameters as a function of thickness reduction were measured. According to trapping model[1] and the method established by J. Baran et al.[2], which determines the specific trapping rate for f.c.c.-metals, we obtained that variation ranges of vacancy concentration and dislocation density were 1×10^{-6} - 3.3×10^{-4} and 3×10^{9} - 2.6×10^{11} cm^{-2} respectively, when the thickness reduction varied from 4% to 25%.

To measure positron lifetime, a conventional fast-slow coincidence system with a resolution of 280ps for cascade γ-rays of ^{60}Co was used. The annihilation radiation γ-rays were detected by a Ge(Li) detector. The resolution of system is 1.3keV for 514keV γ-rays of ^{85}Sr.

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POSITRON AND POSITRONIUM INTERACTIONS AT SURFACES

Allen P. Mills, Jr.

Bell Laboratories, 600 Mountain Avenue, Murray Hill, NJ 07974 USA

Since the pioneering work of Cherry[1] the subject of slow positrons has been intimately connected with surfaces. The first measurements to study eV-energy positrons hitting a metal target in vacuum reported the formation of free positronium in its ground state[2] and first excited state[3]. The relatively high yield slow positron source of Canter et al.[4] permitted subsequent studies in ultra-high vacuum which have given us some understanding of how positrons interact with surfaces.[5] This knowledge has enabled us to make much better slow positron moderators yielding up to 10^2 times higher flux[6]. The higher beam strengths are opening up new possibilities for experimentation on surfaces and solids and for studying the atomic physics of positronium and positron-molecule scattering at low energies. Showing particular promise for surface studies at this time are positron diffraction[7] and tne detection of near-surface disorder[8] using slow positrons.

Our present knowledge of positron and positronium work functions, the positron surface state, positron stopping and positron diffusion will be reviewed. The talk will end with a discussion of what we might do with 10^5 times more slow positrons which should be available soon using exotic sources such as bremmstrahlung-pair-production from electron beam dumps[9] (LINAC, microtron) or large reactor-produced radioactive sources. Finally we may speculate on the possibilities of re-moderation schemes[10] which might allow a 10^8-fold increase in slow positron beam brightness for new experiments in positron scattering and microscopy.

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LOW ENERGY POSITRON DIFFRACTION

K.F. Canter

Department of Physics, Brandeis University, Waltham, MA   02254

The first angle-resolved low energy positron diffraction (LEPD) measurements were made from a Cu(111) surface.[1] Although the angular resolution was poor compared to present LEED standards, the diffracted beam intensity versus incident energy was found to agree well with theory.[2,3]   A study of LEPD from Cu(100) in the same apparatus, but with more precise incident beam alignment, was subsequently carried out along with direct comparisons with LEED.[4] These measurements established that the diffracted beam intensities at energies and angles of interest for surface structure determination range from 10^{-4} to 10^{-3}.   Thus in order to carry out LEPD with resolution comparable to that of LEED, one will typically need a beam flux of 10^5 s^{-1} that can be focussed to 1 mm diameter with an angular spread of 1 degree 100 eV.   With a primary source constraint of 0.5 Ci of Co-58, such specifications can be achieved in principal using the brightness enhancement technique suggested by Mills.[5]

Further improvements in the resolution of LEPD systems are well warranted since, from a theoretical viewpoint, LEPD is superior to LEED for the structural determination of solid surfaces and absorbed overlayers.   At 50 eV, for example, the positron mean free path is 30 percent less than that for electrons[6] and hence LEPD has less contributions from subsurface layers.   This results in an increased sensitivity to the surface and a reduction in the computational time needed for generating theoretical diffraction intensities.   Requirements of long computer times and lack of precise scattering potentials are the major limitations on the precision of LEED work.   Read and Lowy have pointed out that the first layer contraction of W(001) and Mo(001) cannot be determined by LEED mainly because of uncertainty in the choice of the Slater local exchange coefficient to be used for LEED calculations, and such a problem would not be present for LEPD.[3]   Other simplifications in treating LEPD: negligible positron-core electron correlation, reduced spin-orbit polarization effects, absence of appreciable relativistic corrections to positron-ion scattering and reduced multiple scattering[7] for high Z materials.   At present, LEED and LEPD at $\lesssim$ 30 eV are not practical for surface analysis because of the difficulty in treating the many body effects which become significant at these energies.   There may be more impetous for investigating such effects as a result of the observation of a strong (20 percent) first order Bragg reflection peak for $\approx$10 eV positrons incident on Cu(111) and Al(111).[8]   A large negative inner potential for electrons prevents such peaks from being seen for electron scattering from most metals.

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DEFECTS AND DEFECT STRUCTURES IN METALS INVESTIGATED BY SLOW POSITRONS

W. Triftshäuser and G. Kögel

Hochschule der Bundeswehr München, D-8014 Neubiberg, Germany

Monoenergetic positrons of variable energy are used to investigate defects and defect structures in the bulk of metals and alloys and especially configurations in regions close to the surface. The available positron energies are between 150 eV and 28 keV with an intensity of about 10^5 positrons per second. Thus the mean penetration depth of the positrons can be varied from a few 10^{-10} m until 10^{-6} m and hence, for the first time, low energy ion-irradiated (H,He) metal and alloy samples can be investigated by positron annihilation (Doppler broadening). Results are reported for helium-irradiated nickel, copper and aluminium samples as well as for neutron irradiated aluminium and copper and for hydrogen-irradiated nickel. By varying the incident positron energy we observe very pronounced depth profiles of the damaged regions. Significant differences in the positron annihilation characteristics (Doppler broadening spectra) between various defect configurations are detected, especially between voids and helium bubbles. The agglomeration behaviour of helium as a function of annealing temperature and irradiation fluence in α-irradiated samples is being studied.

SUMMARY OF THE CONFERENCE

S. Berko
Department of Physics, Brandeis University
Waltham, MA 02254, U.S.A.

POSSIBLE POSITRON-LATTICE INTERACTION
AT ELEVATED TEMPERATURES OF CADMIUM

W. F. Huang
Department of Physics, University of Louisville
Louisville, KY 40292, U.S.A.
and
L. D. Burton
Jefferson Community College
Louisville, KY 40202, U.S.A.

We have measured the Doppler broadened lineshape parameter and the zero degree angular correlation of the annihilation radiation (DBAR and ZACAR) for Cadmium as a function of temperature ranging from room temperature to near melting point at intervals of about 5°C.

Measurements were performed under two experimental conditions, one with the sample volume free to expand under constant pressure and the other with the sample confined in a molybdenum holder such that its volume remains relatively constant. At each temperature the DBAR and ZACAR measurements were carried out simultaneously. Results from both techniques exhibit typical S-shaped curves. However, up to approximately 170°C, the normalized DBAR and as well as the ZACAR appear to be noticeably larger at constant volume than those at constant pressure. The differences between constant volume and constant pressure furthermore seem to increase with temperature.

We interpret the result as being the manifestation of effects of lattice vibration which causes redistribution of positron wavefunction among atoms and thus, enhances the annihilation of positron in interstitial regions.

ENHANCEMENT FACTORS OF THE ANNIHILATION RATES
OF UMKLAPP TERMS IN METALS

Institut für Kernphysik, Technische Universität Graz
Steyrergasse 4, A-8010 Graz, Austria

A theoretical investigation is presented on the problem how the high momentum components of the annihilation momentum distribution of thermalized positrons annihilating with valence electrons are influenced by interactions of the electron-positron pairs with the lattice of the metal ions.

The main purpose of this paper is a discussion of the so-called Umklapp peaks centered around the reciprocal lattice points.

In the last years, some efforts have been made to calculate the momentum distribution of the annihilating pairs by band-theoretical approaches using the independent particle picture[1]. But despite the fact that these computations include - to a certain extent - correlation effects, ab initio calculations are necessary which evaluate the influence of pair correlations on the annihilation rates of the Umklapp terms.

The first step in this direction was done by a paper of Hede and Carbotte[2]. Our work is a consequent development of their idea.

By using the Green's function method, the correlation effects can be described by summing up some infinite series of ladder diagrams with special insertions due to the fermion-lattice interactions. Each of these ladder series can be evaluated by a numerical treatment of the corresponding integral equation. This procedure is similar to the calculation of the bare ladder sum (see e.g. Kahana[3]).

The result of our investigation is that the enhancement factors of the Umklapp rates are considerably different from those of the central peak, not only concerning their numerical values but also their distribution in momentum space.

In this paper, we present some data giving the enhancement factors of the Umklapp terms, dependent on (i) the mean density of the valence electrons, (ii) the amount and the direction of the annihilation momentum and (iii) the reciprocal lattice vector.

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POSITRON LIFETIME MEASUREMENTS IN INDIUM

W. Puff, P. Mascher, P. Kindl, and H. Sormann
Institut für Kernphysik, Technische Universität Graz,
Steyrergasse 4, A-8010 Graz, Austria

Recently published positron annihilation data have
demonstrated an exceptional temperature dependent behaviour
in the prevacancy region in some metals. In this region the
physics is not yet understood and hence it's uncertain how the
effect should be taken into account in the determination of
monovacancy formation enthalpies. The question if such a pre-
vacancy effect in Indium occurs has not been answered definitely
since the published data are very inconsistent. To solve this
controversy we have measured the positron lifetime in high
purity polycrystalline In samples from 80 K to near the melting
point.

POSITRON ANNIHILATION, MÖSSBAUER-EFFECT AND X-RAY DIFFRACTION STUDIES OF ELECTRODEPOSITED Ni

A. Vértes*, Zs. Kajcsos**, I. Czakó-Nagy*, M. Lakatos-Varsányi*,
H. Leidheiser, Jr.***

Chemistry
*Department of Physical/and Radiology, Eötvös Lorand University,
H-1088 Budapest, Hungary.

**Central Research Institute for Physics, Eötvös Lorand University,
P.O.B. 49, H-1525 Budapest, Hungary.

***Center for Surface and Coatings Research, Lehigh University,
Bethlehem, Pa. 18015, USA.

Structure investigations of electrodeposited nickel were carried out by positron annihilation techniques. Mössbauer-effect and X-ray diffraction measurements were also performed. The samples were produced under different plating conditions yielding stresses in the range of $-10 - +60$ kp/mm^2. The positron lifetime measurements were analyzed in terms of two lifetime components. The first one enables estimations of the concentration of small-size trapping centers while the larger one possibly denotes annihilation at void-like structural imperfections, correlating in size $/\tau_2/$ and concentration $/I_2/$ with the stress applied. Emission Mössbauer spectra using ^{57}Co-doped Ni-samples showed that the magnetic orientation of the deposits was a function of deposition conditions. X-ray diffraction measurements supplemented the Mössbauer measurements in providing information about preferred orientation in the deposits.

INFLUENCE OF AN EXCHANGE CORRECTION ON LIFETIME
AND ENHANCEMENT FACTOR IN KAHANA'S FORMALISM

Z. Szotek

Institute for Low Temperature and Structure Research
Polish Academy of Sciences, 50-950 Wrocław, P.O. Box 937, Poland

The purpose of this paper is to present preliminary results [1] for positron annihilation parameters and screening charge density distributions for r = 2, 3 and 4 obtained when including an exchange correction into Kahana's formalism [2], using an approach proposed by Stachowiak [3]. It is encouraging that these results, although not definite for r_s = 4, anyhow confirm predictions of other authors [4-6], that exchange correlations between screening electrons play an important role in removing a low-density divergence of the total annihilation rate resulting from Kahana's formalism.

An influence of this correction on appropriate parameters b/a and c/a, appearing in Kahana's formula for the momentum-dependent enhancement factor $\varepsilon(p) = a + bp^2 + cp^4$, and total annihilation rates is shown in Tables 1 and 2, respectively. Experimental results [7, 8], the ones of Arponen and Pajanne [5], and those for the static RPA potential [9] are also given for comparison.

Table 1

r_s	Experiment		Results of Arponen and Pajanne			Present Calculations			Results for the static RPA potential		
	b/a	c/a	a	b/a	c/a	a	b/a	c/a	a	b/a	c/a
2	0.13	0.12	3.907	0.13	0.14	3.524	0.19	0.13	3.424	0.17	0.18
3	0.27	0.19	-	-	-	6.998	0.20	0.19	6.066	0.21	0.26
4	0.34[7] 0.16[8]	0.22 0.18	14.08	0.11	0.04	16.02	0.26	0.28	10.94	0.26	0.42

Table 2

r_s	Total annihilation rate $\lambda[10^9 \text{ s}^{-1}]$			
	Experiment	Results of Arponen and Pajanne	Present Calculations	Results for the static RPA potential
2	6.0; 6.2	6.67	6.04	5.87
3	3.76	3.75	3.67	3.24
4	2.9	2.86	3.86	2.69

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POSITRON ANNIHILATION IN ZINC

Z. Pawłowska

Institute for Low Temperature and Structure Research,
Polish Academy of Sciences, 50-950 Wrocław, pl. Katedralny 1,
Poland

The electron-positron pair momentum density distribution in zinc has been computed in the independent particle approximation on the basis of the band structure calculations and the positron wave function.

Results of the application of the selection rule for positron annihilation to the hcp structure are given.

The angular correlation curve was calculated along three main crystallographic directions [100], [001] and [110].

It is shown that taking into account of the enhancement factor proposed recently by Arponen and Pajanne improves the agreement between theory and experiment.
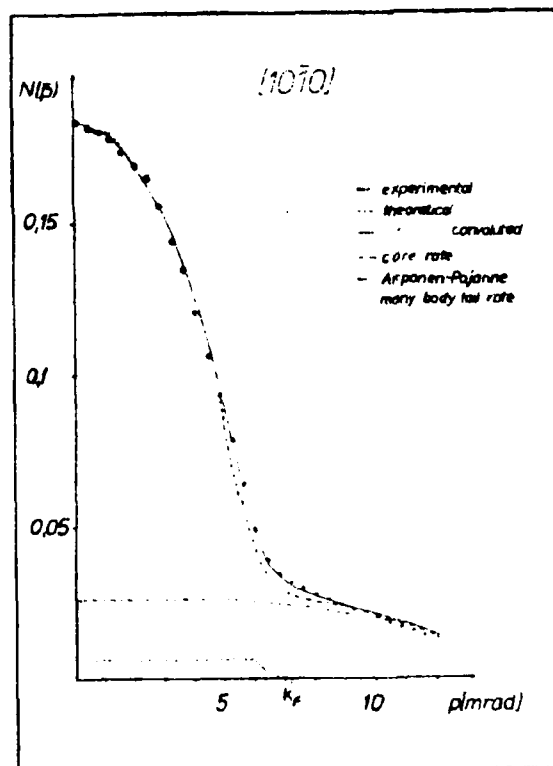
Figure- angular distribution in zinc.

APW CALCULATION OF THE POSITRON ANGULAR CORRELATION IN PD AND PDH[*]

A. Harmalkar and D.G. Kanhere
Department of Physics, University of Poona,
Pune, 411 007, India
and
R.M. Singru
Department of Physics, Indian Institute of Technology,
Kanpur, 208 016, India.

In recent years the electronic structure of metal-hydrogen systems has invoked considerable research interest. Among the metal-hydrogen systems the Pd-H system has received maximum attention both theoretically and experimentally.[1] Earlier the electron momentum distribution in Pd has been experimentally studied by Compton profile measurements and these results have been compared with APW band structure calculations.[2] It would be interesting to make a similar band structure calculation for positron annihilation in Pd and PdH and examine the changes in going from Pd to PdH.

We report here a detailed calculation of the band structure, Fermi surface (FS) and two-photon momentum distribution (TPMD) in Pd and PdH using APW method. The electron wave functions were calculated by using ℓ upto $\ell = 14$ inside the inscribed sphere and 89 plane waves in the interstitial region. The wave function Ψ_+ of a positron in the lowest Γ_1 state is also calculated using the APW method to ensure the correct symmetry and radial behaviour. The results for the band structure for PdH agree with those by Gupta and Freeman[3] and show that a simple protonic model is not valid for PdH. The TPMD, calculated from the APW electron and positron wave functions of Pd and PdH is presented along the important symmetry directions $\langle 100 \rangle$, $\langle 110 \rangle$ and $\langle 111 \rangle$ and the results are discussed in terms of their band structure. The long-slit angular correlation of positron annihilation radiation curves for Pd are compared with experiment. The results for PdH are being reported for the first time and should provide a basis for future comparison with experiment.

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POSITRON ANNIHILATION IN SINGLE CRYSTALS OF
PALLADIUM- AND TANTALUM-HYDRIDES

M. Hasegawa[a], H. Asano[b], and M. Hirabayashi[c]

a)   The Oarai Branch, The Research Institute for Iron, Steel and Other
     Metals, Tohoku University, Oarai, Ibaraki 311-13, Japan
b)   Institute of Materials Science, University of Tsukuba, Sakura, Ibaraki,
     305, Japan
c)   The Research Institute for Iron, Steel and Other Metals, Tohoku University,
     Sendai 980, Japan

Positron annihilation method gives useful information on electronic structures of metal hydrides. We have measured angular correlations and lifetime spectra of positron annihilation in single crystals of $PdH_{0.70}$ and TaH_{015} :

1)   The lifetime in $PdH_{0.70}$ was very sensitive to condition of hydrogen-loading. This shows that lattice defects will easily be introduced by hydrogen intrusion under some conditions, and they will behave as trapping sites for positrons. After several trials of the hydrogen-loading processes, we obtained the sample with the lifetime of about 120 psec which was nearly identical with that in pure palladium. This sample was thought to be nearly free from the lattice defects.

2)   Anisotropies of the angular correlation curves of $PdH_{0.70}$ are similar to those of $Pd_{0.32} Ag_{0.68}$ rather than Pd. This implies rigid-band-model like behavior of change in electronic structure by hydrogen intrusion.

3)   The angular correlation curves of TaH_{015} were very similar to those of Ta. The states near the point N_1', however, were observed to change sensitively by hydrogen intrusion.

MOMENTUM DENSITY FOR POSITRON ANNIHILATION IN RHODIUM

S.B. SHRIVASTAVA and H.P. BONDE
School of Studies in Physics
Vikram University, Ujjain 456 010. India.

With a view to do a systematic study of the electronic structure of 4d transition metals, a band structure calculation of momentum density distribution for positron annihilation in Rh have been performed. The calculations are based on the Hubbard-Mijnarends method.[1] The muffin-tin crystal potentials for Rh have been constructed and used in these calculations. The positron wave function was obtained using the method of expansion of symmetarized plane waves. The calculated momentum densities along the three symmetry directions have been analysed in terms of the band structures and the Fermi surface. The band structure of Rh suggests the occurrence of one hole pocket around X and one around L. However, the hole pocket around X is not surrounded by momentum density contours. Thus the ACPAR may not predict the existence of this hole pocket.

A comparison of band profile in Rh with that in Pd and Ag shows that the band profile in Rh is similar in nature to that in Pd. Both show a broad distribution. But it is different in case of Ag which exhibits a larger parabolic part superimposed on a small broad part because of the NFE character of this metal. Momentum density calculations in other transition metals are under progress.

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INVESTIGATION OF MOMENTUM AND SPIN DESITY OF FERROMAGNETIC NICKEL AND IRON BY POSITRON ANNIHILATION

W. Gerber, G. Dlubek, and O. Brümmer
Sektion Physik der Martin-Luther-Universität Halle-Wittenberg
DDR-4020 Halle (Saale), Friedemann-Bach-Platz 6
German Democratic Republic

The positron annihilation is an important method for the investigation of the electron momentum density (EMD). If a ferromagnetic slugle crystal is magnetically saturated along the direction of an incoming beam of polarized positrons. The shape of the angular correlation curve (AC) will depend on the direction of the magnetization. This makes it possible to study the EMD of the two spin populations of electrons in ferromagnetic materials.

For an investigation of the EMD of ferromagnetic Nickel and Iron we have performed long-slit-angular correlation measurements on seven Nickel and five Iron single crystals using polarized positrons. From these AC's the momentum and spin density are obtained after applying Mijnarends analysis /1/. The experimental determined momentum and spin density were compared with a theoretical one /2, 3/.

The main features of the experimental momentum densities are well reproduced by the theoretical ones. The contour diagram in the (110)-plane shows the presence of the copperlike neck of the Nickel Fermi surface. Also the behaviour of the experimental spin density is well reproduced by the theoretical one in the [110] - and [111] -direction. As it was expected from the theory the spin density of Nickel shows along this directions small high momentum components for $p_z > 14$ mrad. This in contrast to iron, where larger high momentum components in this directions are observable.

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/2/ R. M. Singru, P. D. Mijnarends   Phys. Rev. B9 (1974), 2374

/3/ P. D. Mijnarends   Physica 63 (1973), 235

THE PREVACANCY EFFECTS IN METALS OBSERVED BY POSITRON ANNIHILATION[*]

Lars C. Smedskjaer
Materials Science Division, Argonne National Laboratory
Argonne, Illinois 60439, U.S.A.

At present a controversy exists with respect to the prevacancy effects sometimes observed in supposedly well-annealed metals. The effects manifest themselves as significant deviations from the almost linear temperature dependence of the positron signal predicted by theory (1,2) for temperatures in the prevacancy region.

Two contrasting viewpoints with regard to the prevacancy effects have been suggested. According to one viewpoint, the prevacancy behavior is intrinsic to positron annihilation in perfect metals; thus, the current theories [e.g., (1,2)] have failed to account properly for positron-phonon and/or positron lattice interactions. The contrasting viewpoint suggests that the prevacancy effects are – at least for the major part – extrinsic effects and most likely due to positron trapping in shallow traps.

It is important, with regard to the use of positrons both as probes for defects and electronic structure, to fully understand the prevacancy effects. The present work therefore examines the two contrasting viewpoints and discusses the experimental support presently available for each viewpoint. It will be suggested that the explanation of the prevacancy effects as being due to trapping, should be preferred at present. Furthermore a discussion of the possible positron traps responsible for the prevacancy effects will be given.

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MIGRATION OF VACANCIES IN DEFORMED METALS STUDIED
BY POSITRON LIFETIMES

S. Tanigawa, I. Shinta and H. Iriyama
Institute of Materials Science, University of Tsukuba,
Sakura-mura, Ibaraki 305, Japan

The isochronal annealing behavior in deformed nickel, iron, vanadium, niobium , tantalum, zirconium and other several metals have been studied by the high counting rate measurements of positron lifetimes using a fast timing coincidence system recently developed by Bedwell and Paulus. All the samples were deformed up to 50 % reduction in thickness by rolling at room temperature. Figure 1 shows the results in tantalum. Nearly the same change in τ_M was observed also in nickel and niobium. Figure 2 shows the results of three component analysis after the subtraction of source components. Figure 3 shows the variation of κ_2 and κ_3 with annealing temperature. κ_2 can be considered as proportional to the number of short lifetime defects such as single vacancies and dislocations, and κ_3 to the number of long lifetime defects such as vacancy clusters. On the other hand, the results in iron and vanadium shown in figs. 4 and 5 are quite different.

From the results, it was concluded that vacancies migrate below room temperature in iron and vanadium, at 570K in nickel, 620K in niobium and 570K in tantalum.

In iron and vanadium, the new recovery stage at higher temperatures was found. This stage can be attributed to the annealing stage of vacancy clusters which are formed and grown up during the deformation at room temperature. Detailed analyses of three state trapping model and of the effect of impurity atoms will be presented at the conference.
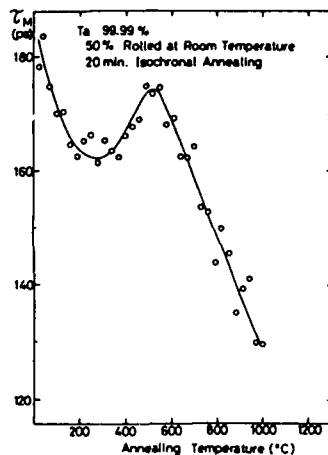
Fig. 1
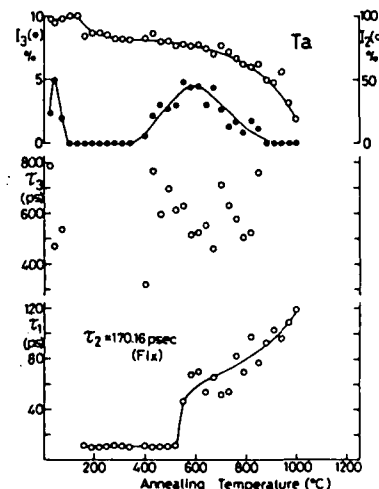
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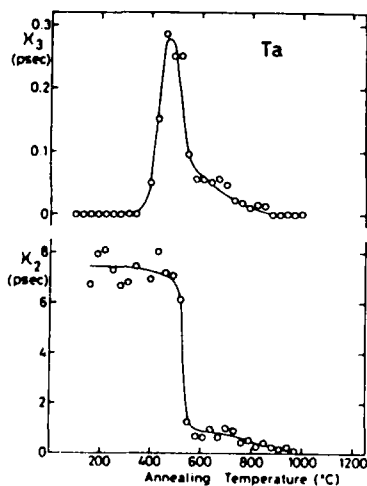
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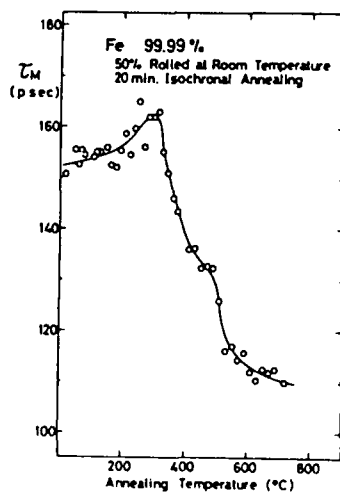
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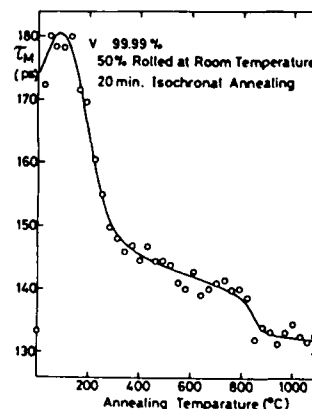
Fig. 5

POSITRON LIFETIMES IN γ- AND α- CERIUM

J.D. McGervey, S.G. Usmar and N. Panigrahi
Department of Physics, Case Western Reserve University, Cleveland, Ohio 44106

O.D. McMasters and K.A. Gschneidner, Jr.
Ames Laboratory, Iowa State University, Ames, Iowa   50011

and

C.-Y. Huang
Los Alamos Scientific Laboratory, Los Anamos, New Mexico   87545

Previous measurements of positron lifetimes in γ- and α-Ce have not shown the effect that would be expected if the phase change were accompanied by the predicted valence change.[1] Because of the rather large uncertainties in these measurements, we have remeasured the lifetime as a function of temperature and pressure, using a hydrostatic pressure cell described previously.[2] Lifetime spectra were obtained at 293 K - 0 kb, 293 K - 9 kb, 293 K - 14 kb, and 77 K - 14 kb. The fitting programs POSFITEXT and EXPFIT gave best fits with a lifetime of (230 ± 3) ps for all spectra. The lifetime spectrometer had a resolution of 300 ps FWHM for ^{22}Na gamma rays, and the source component had a mean lifetime of 800 to 900 ps with an intensity of 7% to 8% for each spectram.

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RECOVERY OF VACANCIES IN IRRADIATED NIOBIUM

J. Yli-Kauppila, P. Hautojärvi, A. Vehanen,
P. Saariaho, H. Huomo, L. Määttänen
Laboratory of Physics, Helsinki University of Technology
SF-02150 Espoo 15, Finland

The annealing behaviour of vacancies in high purity Nb is studied after a 3 MeV electron irradiation in liquid hydrogen as well as after a fast neutron irradiation in liquid nitrogen. The electron irradiation increases the positron lifetime from its bulk value of 122 ps to 170 ps, the latter of which corresponds to saturation trapping at monovacancies. No changes in the lifetime spectra are detected until 380 K, where a longer component abruptly appears increasing up to 420 ps and showing the formation of vacancy clusters. These vacancy agglomerates are very stable surviving even after heat treatments at 900 K.

In neutron-irradiated Nb a longer lifetime component of the order of 200 ps is observed directly after the irradiation indicating that some multiple vacancies are formed within collision cascades. Contrary to the electron-irradiated specimens, neutron-irradiated Nb shows an increase of the positron lifetime already around 200 K. Furthermore the vacancy agglomerates formed at this temperature region anneal out completely below 500 K above which the positron lifetime is equal to that in unirradiated Nb.

The recovery behaviour of vacancies seems to be quite different in the two studied cases. This is probably due to hydrogen impurities in electron-irradiated specimens. The interaction of vacancies and hydrogen is studied and discussed in more detail in neutron-irradiated Nb.

THE POSITRON RESPONSE FROM DISLOCATIONS AND LOOPS IN DEFORMED Mo

B. Nielsen and K. Petersen

Laboratory of Applied Physics II
Technical University of Denmark
DK-2800 Lyngby, Denmark

The recovery of deformed Mo single crystal has been followed by
positron annihilation measurements. A long lifetime component in-
dicates the presence of voids. The short lifetime component contain
the response from vacancies, loops and dislocations. Above stage III
this component only contains the response from loops and dislocations.
Therefore by following the annealing out of this component it is
possible to distinguish between loop and dislocation positron
response. The dislocation density has been followed by TEM inves-
tigations. The results are compared to positron investigation of
the recovery of neutron irradiated Mo, which only contains response
from loops in the short lifetime component.

THE INFLUENCE OF IMPURITIES ON THE RECOVERY
IN STAGES III, IV of 2, 10 AND 40 MeV ELECTRON IRRADIATED Mo, STUDIED BY POSITRONS

H.E. Hansen[1], M. Eldrup[2], S. Linderoth[1], B. Nielsen[1] and K. Petersen[1]

[1] Laboratory of Applied Physics II, Technical University of Denmark
Building 307 - DK-2800 Lyngby, Denmark

[2] Chemistry Department, Risø National Laboratory, DK-4000 Roskilde, Denmark

Isochronal annealings from 50°C to 900°C of 2, 10 and 40 MeV electron irradiated molybdenum were followed with positron lifetime measurements. Two samplesets with different impurity concentrations were used. The impurity concentrations were determined by γ-activation analysis.

The presence of the impurities increases the radiation damage rate and causes a pronounced prolongation of the vacancy migration stage III. Thus the impurities interact with both interstitials and vacancies.

Voidcoarsening and annealing out in stage IV also differs in the two samplesets. This may be due to the difference of impurity - or interstitial loop concentrations or both.

The influence of the irradiation energy on the collision cascades is clearly demonstrated.
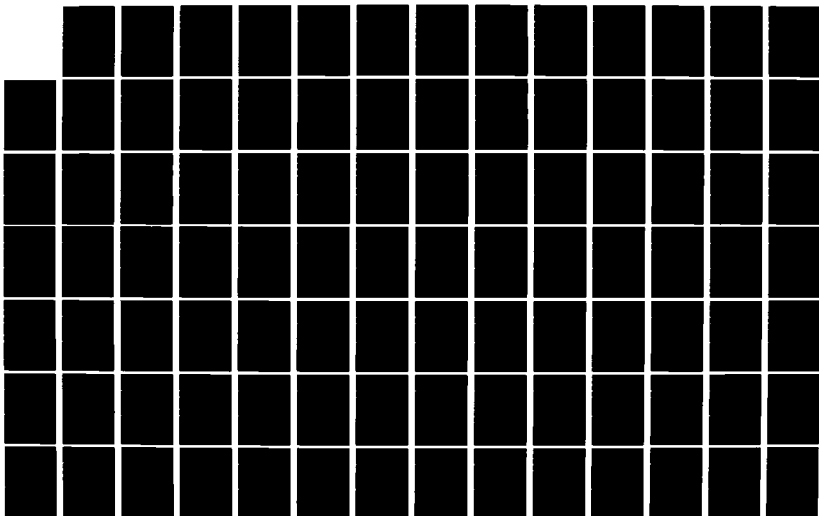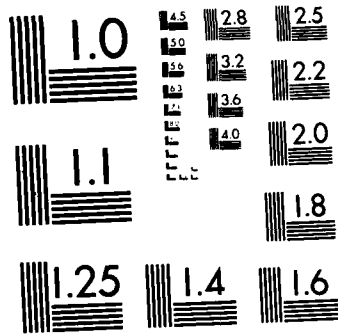
MICROCOPY RESOLUTION TEST CHART

NATIONAL BUREAU OF STANDARDS-1963-A

VOID SHRINKAGE IN HIGH DOSE NEUTRON
IRRADIATED MOLYBDENUM AND TZM

M. Eldrup[a], N.J. Pedersen[a], and J.H. Evans[b]
a) Chemistry Department, Risø National Laboratory,
DK-4000 Roskilde, Denmark.
b) Metallurgy Division, AERE Harwell,
Oxon OX11 ORA, UK.

In a previous investigation by transmission electron microscopy of neutron irradiated high purity molybdenum and TZM (Mo-0.5 wt% Ti-0.1 wt% Zr) a study was made of the influence of irradiation temperature and dose on the void characteristics[1]. A main result was that samples irradiated at $450^{\circ}C$ showed first an increase and subsequently a decrease in void density with increasing dose in the range $1.5-8 \times 10^{22}$ n/cm^2. For TZM even no voids were observed after irradiation to the highest dose. To study this void shrinkage further positron lifetime measurements were made on samples of the two materials irradiated at temperatures of $450^{\circ}C$, $550^{\circ}C$, $600-650^{\circ}C$, and $900^{\circ}C$ to doses of 1.5, 3.5, and 8.0×10^{22} n/cm^2. The presence of voids in all the samples was clearly identified by a long lifetime τ_2 of 458-497 psec, for most samples deviating only a few psec from 475 psec. The intensities I_2 of the void components were in the range 62-89%, except for the samples irradiated at $450^{\circ}C$ to the highest dose, for which $I_2 \simeq 17\%$. Thus the present results show that also in the case where no voids were seen by TEM the positrons clearly detected them. The long lifetime for this TZM sample was 458 ± 6 psec, apparently just below the saturation lifetime for large voids. This is consistent with the voids being below the visibility limit for TEM.

The short lifetimes τ_1 were almost always in the range 150-200 psec, appreciably larger than the bulk lifetime. This indicates that trapping into at least one other type of defect (besides voids) is taking place[2]. Although some evidence supports the idea of trapping at dislocations, we also find a situation where an order of magnitude change in dislocation density leaves the positron parameters virtually unchanged. The reason for the τ_1 lifetime is thus still not settled.

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Positron Lifetime in Deformed Aluminum

Wang Shaojie and Wang Zixiao
Department of Physics, Wuhan University, Wuhan, China
He Yuangin and Yu Weizhong
Department of Engineering Physics, Qinghua University
Beijing, China

Recently, in the field of positron annihilation much attension has been focused on the interaction of positron with defects in Solids, among which, dislocation are practically the most important one, and has been studied widely. The present paper reports the results of a positron annihilation investigation on aluminum deformed plastically by tension.

The specimens used were aluminum plates(99.999 wt%Al) of 0.37 mm in thickness. The tensile strain was in the range of 0.3 to 25.5%. The positron lifetime spectrums were measured by ORTEC 583 fast-fast coincidence system, then analyzed by computer to extract two lifetime components.. The results were τ_b=161ps for bulk state and τ_D=255ps for defect state in good agreement with that of earlier experiments on Al.

Furthermore, using the trapping model we obtained the relationship between concentration of defect and magnitude of strain. The defect concentration increased rapidly with increased of strain in the range of 0.3% to 6%, thereafter, the rate of increase was slowed down and approached a saturation level after 12%. Finally, the specific trapping rate μ_d and dislocation density in stage II of work hardening were calculated. The result μ_d= 0.11cm^2·s^{-1} was obtained with the aid of the formula derived by Dlubek et al. This result was comparable with the theoretically calculated result μ_d=0.3cm^2·s^{-1}. When the tensile strain was 5%, the dislocation density was calculated to be ~2X10^{10}cm^{-2}.

POSITRON ANNIHILATION STUDY OF DEFORMED IRON.

F. Van Brabander, D. Segers, M. Dorikens
and L. Dorikens-Vanpraet

I.N.W., Proeftuinstraat 86, B-9000 Gent, Belgium

Positron annihilation Dopplerbroadening of the 511keV an-
nihilation line and positron lifetimes were measured in de-
formed iron. MRC Marz grade iron and commercial Armco iron
samples were deformed both to 8% and 60% thickness reductions.
In the Armco iron an isothermal annealing effect was seen but
the MRC Marz grade iron samples did not show any such effects.
The isothermal annealing curves for the Armco iron were des-
cribed by an exponential decay function. The time constant
was the same for both deformations. The isothermal annealing
effect is ascribed to the migration of interstitial impuri-
ties, which either decorate defects, making them inefficient
to trap positrons and/or create defects corresponding to
another value for the lineshape parameter. Since probably
more than one trapping centre is responsible for the observed
effect, the isothermal annealing curves were carefully exam-
ined for the presence of more than one decay component but
only one decay constant was observed in all cases. Isothermal
annealing curves were measured at 20C, 27C and 60C. An acti-
vation energy for the migration process was deduced.

Lifetimes and Doppler-broadening were also measured as a
function of the degree of deformation of the MRC Marz grade
iron. It was noticed that saturation trapping already occurs
above 12% thickness reduction, this in contrast to the fcc me-
tals such as aluminium and copper where saturation trapping
occurs at much higher deformations. Positron defect interac-
tion in deformed iron is discussed.

POSITRON ANNIHILATION STUDIES OF MOLYBDENUM IRRADIATED BY PROTONS, OR NEUTRONS OR ELECTRONS

R. H. Howell
Lawrence Livermore National Laboratory
Livermore, California 94550

Both the fluence dependence and recoil energy dependence of traps produced by room temperature irradation of molybdenum have been studied by lifetime and Doppler broadening measurements. Well annealed molybdenum was irradiated by 5 to 19.5 MeV protons, 14 MeV neutrons or 10 MeV electrons. Proton irradiations were performed for fluences of 6×10^{15} cm^{-2} to 10^{18} cm^{-2}. The neutron fluences were between 2×10^{14} cm^{-2} and 9×10^{16} cm^{-2}. Electron irradiations were only done at 6×10^{18} cm^{-2}. By irradiating with so many different sources it is possible to have damage from mainly high energy recoils(14 MeV neutrons), a variable mix of both high and low energy recoils(protons) and mainly low energy recoils(electrons). Positron lifetime and Doppler broadening data were obtained for all of the irradiated samples.

The lifetime spectra were analyzed with a trapping model with two traps and trap lifetimes, and trapping rates were determined. The recoil energy dependence of the trapping rate for the short lifetime trap (lifetime less than 200 psec) indicates that only higher energy recoils produced traps with this lifetime in the proton- or neutron-irradiated samples. The trapping rate of the long lifetime trap (lifetime greater than 400 psec) was correlated with the strength of the low energy recoil production in the proton- or neutron-irradiated samples. The fluence dependence of the trapping rate was smooth but non-linear at the higher fluences. Results of the Doppler broadening measurements are seen to be consistent with the lifetime analysis.

DOPPLER BROADENING OF POSITRON ANNIHILATION RADIATION AROUND FATIGUE CRACKS IN COPPER

S.C. Sharma, R.M. Johnson, Y.J. Attaiyan, L.M. Diana, P.G. Coleman
Center for Positron Studies, Box 19059, UTA Station
The University of Texas at Arlington, Arlington, Texas 76019, U.S.A.

Doppler-broadening spectra have been measured around a fatigue crack in copper. Marked changes are observed in the shape parameters of these spectra in the vicinity of the crack tip. These measurements appear to provide useful information about the plastic zone of a propagating crack.

PRESSURE-DEPENDENCE OF DOPPLER-BROADENED POSITRON-ANNIHILATION LINESHAPES IN COPPER, CADMIUM, ALUMINUM, AND LEAD

R. N. Jeffery
Department of Physics and Astronomy
Wayne State University, Detroit, Michigan 48202 U.S.A.
and
Department of Physics, Mail Code 2508,
Weber State College, Ogden, Utah 84408 U.S.A.[*]

and
E. J. Sendezera
Department of Physics and Astronomy
Wayne State University, Detroit, Michigan 48202 U.S.A.[†]

Doppler-broadened positron-annihilation lineshapes in Cu, Cd, Al, and Pb have been measured at room temperature to 60 kbar. The observed lineshapes were fitted to a function consisting of Gaussian (core) and parabolic (valence electron) components, convoluted with the detector resolution function (1.25 keV, FWHM), plus background. Core fractions (CF) were determined from the ratio of the area under the Gaussian component to the combined Gaussian and parabolic areas. In addition, the more readily determined S parameter was computed from the raw spectra as the area under a central region divided by the area under the whole line. Increasing pressure causes the lattice to contract, the core fraction to increase, and the S parameter to decrease. Both CF and the S parameter change in proportion to the fractional volume change. The zero-pressure core fractions, CF(0), agree quite well with other works. These are: Cu 0.55, Cd 0.53, Al 0.18, and Pb 0.35. The proportionality between the CF change and the volume change is approximately one for cadmium and lead and two for copper and aluminum. The proportionality between the S parameter changes and volume change, $\beta_f p$, is approximately one for cadmium, aluminum, and lead, and two for copper. The analogous thermal expansion coefficients, $\beta_f T$, in the literature generally agree with $\beta_f p$ around the value unity except for copper.

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[*] Present address.

[†] Current address: University of Malawi, Blantyre, Malawi, AFRICA.

CORRELATION EFFECTS FOR LOCALIZED POSITRON STATES

M. Manninen
SIN, Villigen, 5234 Switzerland
and
R. M. Nieminen
Department of Physics, University of Jyväskylä,
40720 Jyväskylä, Finland

A two-component density-functional theory is developed to handle electron-positron correlations for localized positron states. The specific aim is to evaluate the positron-induced distortions in the defect electron structure and the positron distribution in an accurate, self-consistent fashion. The development draws on the analogy with the electron-hole plasma, and the results obtained for that system are exploited in construction of the necessary correlation energy functionals. As a test example, positron trapping at a vacancy in jellium metal will be treated in detail.

DOPPLER-BROADENING MEASUREMENTS IN THERMAL EQUILIBRIUM
IN ALPHA-IRON.

D.Segers(*), L.De Schepper(**), L.Dorikens-Vanpraet(*),
M.Dorikens(*),F.Van Brabander (*), G.Knuyt(**),
J.Van Oppen(**),L.Stals(**) and P.Moser(***)

(*)   I.N.W., Proeftuinstraat 86, B-9000 Gent, Belgium
(**)   Materials Physics group, Limburgs Universitair Centrum,
       B-3610 Diepenbeek, Belgium
(***) Section de Physique du Solide, Centre d'Etudes
       Nucleaires de Grenoble, 85X, 38041 Grenoble Cedex,
       France

Positron annihilation Doppler-broadening measurements on
alpha-iron in thermal equilibrium were carried out. A sealed
source technique was used. S-parameter and W-parameter re-
sults were obtained for extremely pure iron (total intersti-
tial content below 5at ppm) and for iron containing well con-
trolled amounts of interstitial impurities.

The results were analyzed by taking into account the
trapping of positrons into vacancy-carbon pairs besides
mono-vacancies. The influence of this mechanism on the onset
temperature for vacancy trapping is discussed. Our results
are compared with the experimental results in literature.
Complications for the determination of the vacancy formation
enthalpy in alpha-iron are discussed.

ON THE ZERO POINT MOTION OF POSITRONS
TRAPPED BY DEFECTS IN VARIOUS METALS

M. McGetrick[*]. C. Coleman[†], A.E. Hughes[†]
and P. Rice-Evans[*].
* Department of Physics, Bedford College, University of London,
Regent's Park, London, NW1 4NS.
† Materials Development Division, A.E.R.E., Harwell, Oxfordshire.

The procedure of fitting Doppler-broadened line shapes of annihilation radiation with parabolic and Gaussian components, with an additional broadening to account for positron motion [1] has been applied to defect trapping in a number of metals including copper, aluminium, titanium, iron, nickel, etc. Thermally induced vacancies and defects induced by plastic deformation have been investigated. In all cases it is found that the inclusion of positron motion improves the fitting. An analysis of the results suggests that the traps induced by plastic deformation have a point-like character.

Reference
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A DETAILED DISCUSSION OF POSITRON ANNIHILATION LINE SHAPE ANALYSES AND A COMMENTARY ON THE TRAPPING MODEL

T. Chaglar
Higher Technological Institute Gazi-Magosa,
Mersin 10, Turkey.

L. Rice-Evans and A.A. Berry,
Department of Physics, Bedford College.
University of London.
Regent's Park, London, NW1 4NS, England

Abstract: The use of line-shape parameters in the trapping model is described and two models which seek to explain the temperature dependence of line-shape parameters are discussed. A review is given of reported results of positron annihilation on cadmium and we report results arising from two distinct specimens of single crystal cadmium. A commentary is made on the trapping model in the light of these reported results and a detailed momentum profile analysis presented here.

POSITRON STATES IN SOME LIQUID METALS
IN COMPARISON WITH THE TRAPPED STATE AT VACANCIES

Y. Kishimoto and S. Tanigawa
Institute of Materials Science, University of Tsukuba,
Sakura-mura, Ibaraki 305, Japan

Positron states in liquid metals are not clearly understood.   It has been well known that in some metals positrons are trapped by thermal vacancies, but in the others can not be trapped.   This means that the trapping probability of a vacancy μ_v varies between $10^{12} sec^{-1}$ and $10^{16} sec^{-1}$ depending on the species of metals.   Furthermore, the essential problem remains yet unanswered as for the positron trapping model.   That is, which model is probable between a strong localization model and a weak localization one.   The conventional positron annihilation techniques have not yet given a clear answer to these problems. On the other hand, the new technique, positron age-momentum correlation measurements, would provide a useful information about the separation of several annihilation modes.   In the present paper, this correlation was measured in both liquid and solid states of gallium and indium.

Figure 1 shows the results in gallium.   In solid region, the lifetime was independent of momenta.   This fact means that positrons annihilate from only one state, maybe a free state.   In liquid region, a minimum of the lifetime was found where the momentum equals to zero.   This a evidence of the coexistence of at least two annihilation modes.   One of them has the shorter lifetime and the narrower momentum didtribution, and the other has the longer lifetime and the broader momentum distribution.   Figure 2 shows a temperature dependence of total lifetime in indium.   It was firstly found that lifetimes decrease upon melting.   Figure 3 shows resolved lifetimes in each energy channel of Doppler broadening.   I2 means the source component.   A dashed curve indicates the expected values under the assumption of a strong localization extreme.   In the present experiment, the selected energy range was too narrow to decide which model is probable.   The correlation measurement in the wider range of annihilation energy is in progress.
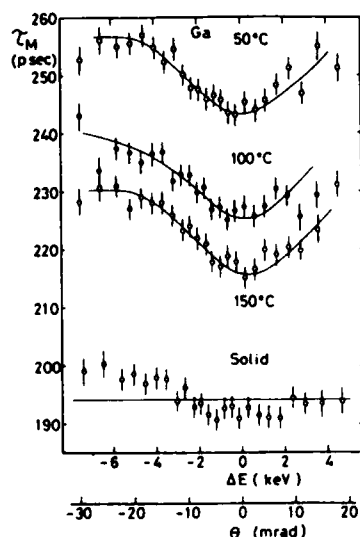
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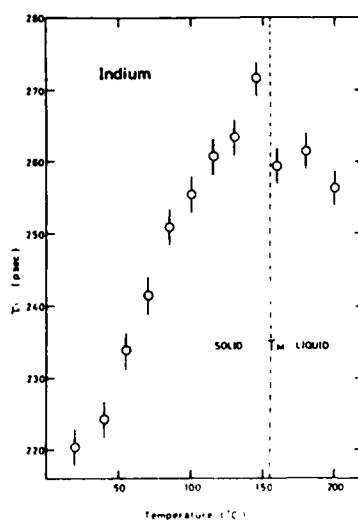
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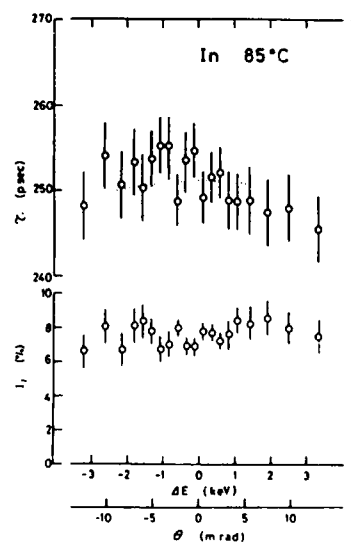
Fig.3

QUANTITATIVE STUDIES OF QUENCHED-IN VACANCIES
IN ALUMINUM BY POSITIVE MUONS

M. Doyama,[#*] R. Nakai,[#*] R. Yamamoto,[#*] S. Tanigawa[*#$], Y.J.Uemura[**#] and T.Yamazaki[**#]

* Department of Materials Science, Faculty of Engineering
  The University of Tokyo, Hong, Bunkyo-ku, Tokyo 113 Japan

** Department of Physics, Faculty of Science, The University
   of Tokyo, Hongo, Bunkyo-ku, Tokyo 113 Japan

TRIUMF, University of British Columbia, Vancouver, B. C.
  Canada V6T 2A3

A positive muon is an isotope of a positron. It is well known that positrons are trapped by vacancies. Therefore positive muons should be trapped by vacancies in metals. This paper shows that the muon experiments can be used to study vacancies in pure aluminum.

99.9995% pure aluminum sheets (25 x 25 x 0.5 mm^3) were rapidly quenched from 853 K , 673 K, 600 K, 550 K and 500 K to a mixture of HCl and water kept at 200 K. These aluminum sheets were kept in liquid nitrogen.

The muon spin relaxation rates in the specimens were measured by zero field relaxation method. The trapping model was quantitatively applied. The diffusion rate of positive muons in pure aluminum was determined. The diffusion rates obey the Arrhnius law between 140 K and 200 K. The activation energy for a muon to diffuse in this temperature range is found to be 0.039 ± 0.015 eV. Below 140 K, the diffusion of positive muons deviates from the Arrhenius law due to the quantum diffusion.

Changing the quenching temperatures, the formation energy of a vacancy in pure aluminum was determined to be 0.68 ± 0.03 eV. The muon spin research can be used to study vacancy type defects quantitatively.

$ Present address: Tsukuba University

MUON SPIN RELAXATION ANALYSIS BY TRAPPING MODEL WITH DETRAPPING

T. Hatano*# Y. Suzuki*# T.Natsui*# M. Doyama*#
Y. J. Uemura+# T.Yamazaki+# J. H. Brewer#

*Department of Metallurgy and Materials Science, Faculty of engineering
 The University of Tokyo, 7-3-1 Hongo Bunkyo-ku Tokyo 113 Japan
+Department of Physics, Faculty of Science, The University of Tokyo
 7-3-1 Hongo Bunkyo-ku Tokyo 113 Japan
#TRIUMF University of British Columbia, Vancouver, B.C. Canada

The positive muon is a powerful prove for the study of microscopic crystal structures according to the muon trapping to the lattice defects. In this point of view, it is quite important to take account in the dynamic properties of muon in the crystals. A precise expression is obtained for muon spin relaxation function under zero field including trapping and detrapping. This expression is a extension of the method by Hayano et.al. (1), which is considered the hopping of muons.In the case of Aluminum, muons are delocalized down to 1K, and the dynamic property is likely to be explained by trapping and detrapping model. The diffusion of muons is quite sensitive to the lattice defects such as quenched-in vacancies(2,3) and impurities(4). But observed relaxation rates are smaller than that of calculated from Van Vleck values. Several reasons are proposed to explain the experimental data, such that muons are not trapped at vacancy sites but itinerate around vacancy sites(2,3) or the diffusion of muons is suppressed by the strain field around impurities(4). Diffusion and detrapping of the muon lead the relaxation rates smaller. Therefore we calculated the precise values for muon spin relaxation function under the zero field including trapping and detrapping. Actual relaxation function is written as follows by stochastic theory,

$$G(t)= e^{-\nu_1 t} g_f(t) + \int_0^t \nu_1 e^{-\nu_1 t_1} g_f(t_1) e^{-\nu_2(t-t_1)} g_t(t-t_1) \, dt_1$$

$$+\int_0^t \nu_2 e^{-\nu_2(t-t_2)} g_f(t-t_2) dt_2 \int_0^{t_2} \nu_1 e^{-\nu_1 t_1} g_f(t_1) e^{-\nu_2(t_2-t_1)} g_t(t_2-t_1) dt_1 + \ldots$$

$$F(s)= \sum_{n=0}^{\infty} f_f(s+\nu_1)[1+\nu_1 f_t(s+\nu_2)](\nu_1\nu_2 f_f(s+\nu_1) f_t(s+\nu_2))^n$$

$$= \frac{f_f(s+\nu_1)\,[1+\nu_1 f_t(s+\nu_2)]}{1-\nu_1\nu_2 f_f(s+\nu_1)\,f_t(s+\nu_2)}$$

where $g_f(t)$ is the relaxation function of delocalized muons, $g_t(t)$ relaxation function of trapped muons, ν_1 trapping rate of delocalized muons, ν_2 detrapping rate of trapping muons. $F(s)$, $f_f(s)$, $f_t(s)$ are the Laplace transforms of $G(t)$, $g_f(t)$, $g_t(t)$, respectively. Using this expression we can distinguish the effect of muon diffusion and the nature of the trapping sites.

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POSITRON ANNIHILATION MEASUREMENTS OF VACANCY FORMATION IN TUNGSTEN[*]

L. C. Smedskjaer, M. K. Chason, and R. W. Siegel
Materials Science Division, Argonne National Laboratory,
Argonne, Illinois 60439, U.S.A.

Doppler-broadening measurements of vacancy formation in tungsten are being carried out over the temperature range from 300 K to just below its melting temperature of 3695 K. The high-purity tungsten sample is electron-beam heated and maintained in an ultra-high vacuum during the measurements. Sample purity is further maintained through the use of $\sim 10^{14}$ ion-implanted ^{58}Co atoms for the positron source.[†] The Doppler-broadening data, F(T), will be used to obtain a value for the monovacancy formation enthalpy that can be compared with previous results from quenching (3.5 eV) and positron annihilation (4.0 eV) investigations. Beyond this, considerable emphasis is being placed upon obtaining high-quality data from the high-temperature parts of the sigmoidal F(T) curve, in order to gain additional insight regarding the high-temperature equilibrium vacancy ensemble in tungsten. These results will be discussed in the light of our present knowledge of vacancy defects in tungsten obtained from previous self-diffusion and quenching studies.

A POSITRON ANNIHILATION STUDY OF THE EQUILIBRIUM VACANCY ENSEMBLE IN ALUMINUM[*]

M. J. Fluss[‡†], S. Berko[‡], B. Chakraborty[†], K. Hoffman[‡],
P. Lippell[‡], and R. W. Siegel[†]

[‡]Department of Physics, Brandeis University,
Waltham, Massachusetts 02154, USA
[†]Materials Science Division, Argonne National Laboratory,
Argonne, Illinois 60439, USA

Positron annihilation spectroscopy of vacancies in Al has been carried out under thermal-equilibrium conditions, using both one- and two-dimensional angular correlation of annihilation radiation (1D- and 2D-ACAR) techniques. Measurements have been made on oriented single-crystal Al samples, maintained under ultra-high vacuum, in the temperature range of 295-920 K, and for several momentum-integration directions. In addition, the annihilation characteristics of a positron from both its monovacancy- and divacancy-trapped states have been calculated self-consistently within a supercell, with the inclusion of many-body enhancement effects. The measured 1D- and 2D-ACAR spectra for positrons annihilating in essentially defect-free Al and in Al containing vacancies will be compared with one another, and with the results of the theoretical calculations. The anisotropies and temperature dependences in the experimental results will be presented, and compared where possible to the theoretical results in an attempt to obtain the first direct spectroscopic information regarding the presence of divacancies in equilibrium at high temperatures in Al. Finally, the possibility to extract detailed localized electronic-structure information regarding vacancy defects in metals using these techniques is being explored.

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A POSITRON STUDY OF THE EFFECT OF W, As, Sb, and Ti ON THE ANNEALING OF DEFECTS IN COLD-ROLLED Ni

G. Dlubek, N. Meyendorf, and O. Brümmer
Sektion Physik der Martin-Luther-Universität Halle-Wittenberg
DDR-4020 Halle (Saele), Friedemann-Bach-Platz 6
German Democratic Republic

Defect concentrations and annealing processes in plastically deformed Ni were investigated by our group in past /1 to 4/. In the present work we have measured the peak height of 2γ -angular correlation curve during time-linear heating of 90 % cold-rolled Ni dilute alloyed with W, Sb, As and Ti (0.03 to 1.4 at. %). The results show that small amounts of foreign elements effect in very different manner the annealing behaviour of cold-rolled Ni. Beside a shift of the recrystallization to higher temperatures, the recovery of vacancies is more or less modified. In pure Ni the vacancies disappear between room temperature and 100 °C. The additions of W to Ni shifts the annealing of vacancies slightly to higher temperatures. However, in As- and Sb-doped Ni a strong increase of the peak height is observed which starts at about 100 °C. The increase is attributed to the formation of a large number of three dimensional vacancy clustert nucleated at As or Sb atoms /4/. The diffent effect of W, As and Sb correlates with different binding energy of these elements to vacansies in the Ni matrix.

The behaviour of Ti-doped Ni differs from that of the other samples. In contrast to W-, As- and Sb-doped Ni, the degree of deformation (ε = 20 to 90 %) influences only weakly the measured annealing curves. Investigation by transmission electron microscope and positron lifetime measurements support the picture that positrons are localized at small Ti-rich clusters (precipitates).

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HIGH-RESOLUTION POSITRON LIFETIME AND DOPPLER BROADENING MEASUREMENTS OF POSITRON TRAPPING AT DISLOCATIONS IN COPPER

S.C. Sharma, Y.J. Attaiyan, R.M. Johnson, L.M. Diana, S.Y. Chuang,P.G.Coleman
Center for Positron Studies, Box 19059, UTA Station
The University of Texas at Arlington, Arlington, Texas 76019, U.S.A.

High resolution lifetime and Doppler broadening spectra have been measured for positrons annihilating in copper single crystals as a function of the density of dislocations. Copper single crystals were grown by the modified Bridgeman technique and oriented along 111 faces to permit the formation of etch-pits. Dislocations were introduced by applying uniaxial tensile loads and dislocation densities were estimated from the measurements of the etch-pits and the resolved shear strain. The behavior of the annihilation parameters, obtained from unconstrained analyses, as a function of the density of dislocations, will be discussed.

HIGH AND LOW AMPLITUDE FATIGUE IN COPPER
SEEN BY POSITRON ANNIHILATION

L. P. Karjalainen, T. Judin and M. Karras
University of Oulu, 90570 OULU 57, Finland

The distinction has been expressed previously between high and low amplitude behavior of copper, a discontinuity in fatigue life curves, difference in dislocation structures, stored energy and in type of hardness dependence on stress amplitude are reported. Here the positron annihilation is used to study this difference.

The mean positron lifetime (τ) and Doppler broadening lineshape S-parameter are determined simultaneously and compared to microhardness for annealed polycrystalline pure copper during fatiguing into saturation stage at high amplitude (5 x 10^3 cycles at 0.0034) and at low amplitude (3.7 x 10^5 cycles at 0.0010) and during isochronal annealing (30 min from 470 to 770 K with a step of 50 K) of fatigued structures. Cold rolled copper is tested for reference (2 x 10^5 cycles at 0.0020).

During cycling strain hardening causes increase in τ and S-parameter in confidence with hardness in annealed material. At the saturation stage τ and S-parameter are higher for high amplitude structure (dislocation cells) than for low amplitude structure (dipole patches) in spite of lower hardness of the former. This may indicate higher defect densities, though their very uneven distribution in cell structure offers less resistance to long-range dislocation motion. The difference remains during annealing throughout the recovery stage which can be distinguished from the region of the disappearance of dislocations and dipoles for both structures, as shown in the figures below.

A different response of τ and S-parameter on fatigue cycling is observed for cold rolled copper, the former increasing and the latter decreasing at the stage of cyclic softening. An anti-recovery stage is revealed at 570 K by both τ and S-parameter, but not indicated by hardness variation. The possible causes are considered briefly.
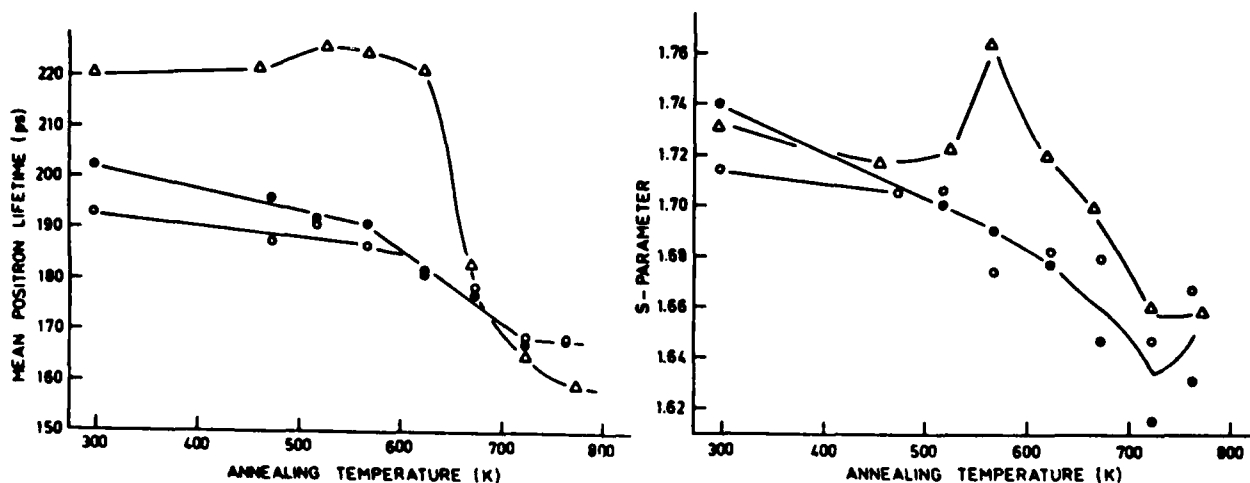
Figures. Annealing characteristics of the lifetime and S-parameter after fatigue cycling ($\bullet$ ± 0.0034, 5 x 10^3 cycles, o ± 0.0010, 3.7 x 10^5 cycles, $\triangle$ cold rolled, ± 0.0020, 2 x 10^5 cycles).

DEFORMATION EFFECT ON POSITRON ANNIHILATION
IN TITANIUM ALLOYS

I.Ya.Dekhtyar, R.G.Fedchenko, A.I.Kupchishin, K.M.Mukashev,
V.A.Rafalovsky
Institute of Metal Physics, Acad.Sci.UkrSSR,Kiev-142, USSR

The method of angular correlation of annihilation photons was used to study the interaction between positrons and deformation defects in Ti-Al, Ti-Ir, Ti-Ge and Ti-Sn alloys. Deformation ($\varepsilon \approx 50\%$) causes abnormally large changes in the annihilation characteristics: $F = S_p / S_g$ (S_p and S_g are the areas under the parabolic and gaussian parts, respectively) and θ_F (the angle corresponding to the Fermi momentum). The growth of F and the decrease of θ_F is interpreted as the result of $\alpha \rightarrow \beta$ polymorphic transformation initiated by the plastic deformation creating stacking faults with the structure of bcc-phase in the matrix of hcp-phase. The trapping center size was estimated as several nm. Correlation is observed between the F variation and the parameter which defines the lattice instability.

It is concluded that the trapping center structure in deformed alloys on Ti base is related to the defects of microvoid type, such defects being produced in the neighbourhood of β-phase particles.

VACANCY LONG RANGE MIGRATION IN AUSTENITIC $Fe_{59}Cr_{16}Ni_{25}$

C. CORBEL[*], O. DIMITROV[**], P. MOSER[***]

[*] Section d'Etude des Solides Irradiés (CEN-FAR), 92260 Fontenay-aux-Roses France

[**] Centre d'Etudes de Chimie Métallurgique (CNRS), 94400 Vitry, France

[***] Section de Physique du Solide (CEN-G), 85-X, 38045 Grenoble, France

Positron lifetimes in 20 K electron irradiated $Fe_{59}Cr_{16}Ni_{25}$ stainless steel, prepared from pure components, are measured at 77 K at the end of isochronal annealings (30 mn/25 K) between 77 K and 670 K. The composition of pure austenitic Fe-Cr-Ni alloys is selected to have a f.c.c. single phase stable at low temperature. In specimens irradiated at doses $2.5 \cdot 10^{18}$ the trapping of the positron is saturated at 77 K. The positron lifetime in the defect is 180 ps. This defect corresponds probably to single vacancies (several configurations are possible for single vacancies and 180 ps is an average value in the different configurations). Single vacancies are observed up to 270 K. Above this temperature defects with a volume larger than the vacancy volume appear. Their volume growths up to 320 K. The further evolution of the new defects indicates that several kinds of vacancy clusters are in equilibrium. The clusters disappear in two stages. Between 300 K and 400 K there is a rearrangement of the structures. The size distribution is shifted to smaller sizes and the positron lifetime in the defects decreases from 215 ps to 190 ps. Above 500 K, the defects are no more stable and at 650 K they have completely dissappeared. A single positron lifetime equal to 112 ps, as before irradiation, is then measured.

Above 270 K, the formation of vacancy clusters show that vacancies are performing their long range migration. This result is consistent with tne study of electrical resistivity recovery by O. Dimitrov et al. and shows that the vacancy long range migration occurs in the second stage of resistivity recovery observed between 260-400 K.

The average volume by cluster in $Fe_{59}Cr_{16}Ni_{25}$ is smaller than in pure iron where the highest values of τ_2 are about 300 ps.

EXAMINATION OF HYDROGEN EMBRITTLEMENT IN STEEL BY POSITRON ANNIHILATION

Yu Weizhong, Yao Jianxi, He Yuanjin, Xiong Jiajiong

Department of Engineering Physics of Qinghua University,
Beijing, China

and

Zhang Jinzeng, Shen Wanci, Gu Jialin, Chen Nanping

Department of Mechanical Engineering of Qinghua University,
Beijing, China

The behavior of positrons in metals is in some aspects analogous to hydrogen. In the field of hydrogen embrittlement studied by positron annihilation some intresting results had been obtained in the previous works by Doyama, Alex and Byrne. Because of the complexity of the defects in steel and the shielding effects of protons on the effective charges of defects, the analysis of the experimental data is rather difficult. Research in this field has not been developed rapidly.

To overcome the difficulties mentioned above, we have rearranged the experimental procedure carefully. Besides the measurements of differently charged states, the measurments of initial states before charging and the measurments of hydrogen - discharged states were added. The times and temperatures of charging, aging, discharging, and measurment of positron lifetimes were all exactly controlled. Then, the conclusion was reached that the positron trapping rates of dislocations in 01rl3Ni8Mo steel are approximately proportional to the density of charging current.

The effects of stress on hydrogen embrittlement have also been examined. The results of measurments of differently loaded and unloaded samples suggest that stress may enhance the hydrogen embrittlement strongly.

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POSITRON ANNIHILATION STUDY OF AGING PHENOMENA IN MAGNETIC ALLOYS
SmCo$_5$

He Yuanjin, Yu Weizheng, Xiong Jiajiong

Department of Engineering Physics, Qinghua University,
Beijing, China

and

Xie Hongzu, Cheng Minjie, Liang Shanglan

Baotou Metallurgical Institute, Baotou, China

That positron annihilation technique (PAT) is sensitive to aging
and precipitation phenomena has been proved in some typical alloys,
such as aluminium based alloys. But more efforts have to be made in
order to apply PAT to the study of unknown aging or precipitation pro-
cesses. Some results obtained from PAT study of aging phenorena in
magnetic alloys SmCo$_5$ are reported here. The microstructure of this
alloy and its aging behavior are not very clear yet.

Position lifetime measurements have been made for three sets of
alloys SmCo$_5$, the samarium concentrations of which are different
slightly. The specimens were classified into two groups. One group
of specimens has undergone isochronic annealing, and another isother-
mal annealing. The annealing temperatures are from 30 to 740°C, and
the annealing times are from 10 to 480 min. The results of PAT then
were compared with that of transmisson electron microscope (TEM) and
of resistance measurments.

Very complex aging phenorena were observed. There exist two kinds
of machanisms for the aging processes in the alloys SmCo$_5$. One is
called "low temperature aging", which can occur at a temperature as low
as 50°C, and another "high temperature aging", which can occur
significantly only at about 600°C.

The mechanism of "high temperature aging" is similar to precipita-
tion of a new phase, which accompanied by an increase or a decrease
of the positron bulk lifetime τ_b. The effects on τ_b by different
precipitation phases, Sm-riched or Co-riched, are different. About
this difference some discussions have been made.

The "low temperature aging" was rather peculiar. The trends of
variations of positron parameters were affected by neither the
constitutional deviations, nor the annealing temperatures (50°C, 200°C,
400°C), but were determined mainly by annealing time. The possibility
of using positron as a micro probe to aging phenomena will be
discussed.

The Study of Aging in Multicomponent
Aluminum Based Alloy by Positron Annihilation
Wang Shaojie and Wang Zixiao
Department of Physics, Wuhan University, Wuhan, China
He Yuangjin and Yu Weizhong
Department of Engineering Physics, Qinghua University
Beijing, China

The kinetics of isothermal aging and the effect of defor-
mation on aluminum-based alloy($\sim$5.5wt% Zn, 2.5wt.%Mg, 1.5wt
%Cu, 0.2wt.%Cr, remainder Al) were investigated by positron
Annihilation. The later has been rarely reported up to now.

The specimens were solution-heat-treated at 480°C follwed
by water-quenching and then aged at $130\pm1.5^{\circ}$C for different
time interval from 30 to 960 min. One set of samples was
rolled 6% before aging, and the rest undeformed. Positron
lifetime was measured at room temperature in compared with
hardness measured in parallel.

The fact that the positron mean lifetime of specimen
aged at room temperature was longer than that of pure aluminum
proved that G. P. zone provided efficient trapping sites for
positrons. This may be explained by pseudopotential theory.
According to Dlubek et al., the positron pseudopotential
difference V_0 are 0.4ev for Al-Zn alloy and 1.7ev for Al-Mg
alloy. The positive value of V_0 means a positron
affinity for Zn and Mg over Al.

For water-quenched specimen, there were two maxima of
positron mean lifetime at about aging of 4 hours and 8 hours.
The former might be due to the structure change of the initial
stage of G. P. zone. The coherent effect of G. P. zone with
matrix led to hardening of the alloy. So there was a peak value
of hardness at the same aging time. The maximum at aging of
8 hours was suggested as corresponding to the formation of
the transition phase η'.

For rolled specimen, there were some remarkable differences.
In the early stage of aging, the positron mean lifetime was
less than that of the water-quenched specimen, the aging effect
weakened and the aging kinetics delayed. These might be
attributed to the precipitation of vacancies and the nucleation
of coarser precipitates on dislocations.

The Study on Defect in α-LiIO$_3$ Single Crystal under the Action of an Electrostatic Field by Positron Annihilation

Huang Mao-rong,   Yin Ding-zhen
Institute of High Energy Physics, Acadimia Sinica,
Peking,   China

The change of vacancy in α-LiIO$_3$ single crystal under the action of an electrostatic field was investigated by positron annihilation lifetime spectra. The time spetra were able to be divided into three components, that is τ_1 :0.20 – 0.25 ns, τ_2:0.30 – 0.50 ns, and τ_3:1.6 – 2.0 ns. Their intensities are I_1: 50 –93 %, I_2: 50 – 6 % and I_3: 1–2% respectively. The range of electrostatic field strength, E, used was from 300V/cm to 1900V/cm. Although the lifetime have a very complicated relation with E. They completely correspond with a trapping model in which the escape rate can not be neglected. The capture rate and escape rate under different E were calculated. The lifetime for perfect α-LiIO$_3$ single crystal, τ_f=0.24ns, was obtained. The complicated relation of the lifetimes with E was considered to be due to the migration of vacancies and the interaction of various defects. The lifetime change we obtained experimentaly might have the same mechanism as that obtained by other experiments, say X-ray topography.

Investigation of the Recovery of Deformed Iron by Positron Annihilation

Cao Chuan, Wang Yun-yu,   Xiong Xing-min
Institute of High Energy Physics,Acadimia Sinica,
Peking,   China

Jiang Jian,   Xiong Liang-yue
Institute of Metal Research,Acadimia Sinica,
Shenyang,   China

Abstract

The recovery behavoir of the 60% deformed iron
in various stages of isochronal annealing have been
investigated by positron annihilation technique.
The experimental results showed that both the
average life time and the line shape parameter S
of the positron annihilation may be expressed as
the function of annealing temperatures. Life time
τ_f of the positron annihilation in the perfect
lattice was found to be 111 $\pm$ 1 ps,   whereas τ_d
in the defect to be 162 $\pm$ 1 ps.   Trapping rates
and τ_t were calculated, these values are in good
agreement with that expected by trapping theory.
From calculation it was obtained that the range
of fractional concentration of defect trapping
positron is $10^{-7}-10^{-4}$.

Determinating the Change of Concentration
of Vacancy and Dislocation by means of PAT
in plastic deformed Iron

Xiong Lian-yue,   Jiang Jian

Institute of Metal Research, Acadimia Sinic,
Shenyang, China

Cao Chuan, Wang Yun-yu, Xiong Xing-min

Institute of High Energy Physics, Acadimia Sinica,
Peking, China

Abstract

The change of concentration of vacancy and dislocation in 60% plastic deformed iron have been studied by positron annihilation technique. The experimental results show that the trapping rate of positron in defect may be expressed as the function of isothermal annealing time; vacancy and dislocation are the main defects that trapping positron. The changes of concentration of vacancy with isothermal annealing time obey the relation $C_v(t)=C_v(0)e^{-kt}$, while dislocation obey the relation $C_d(t)=C_d(0)e^{-(t/\tau)^n}$.

The recovery active energy of vacancy and dislocation calculated are 12.5kcal/mole and 75 kcal/mole, respectively, which agree with that determinated by other ways.

POSITIVE MUON BEHAVIOR IN QUENCHED ALUMINUM DILUTE ALLOYS

M. Doyama*#,T. Hatano*#,T.Natsui*#,Y. Suzuki*#, Y. J.Uemura**#,T. Yamazaki**#

and J. H. Brewer#

* Department of Metallurgy and Materials Science
  Faculty of Engineering, The University of Tokyo
  7-3-1 Hongo, Bunkyo-ku Tokyo 113 Japan

** Department of Physics, Faculty of Science, The University
   of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113 Japan

TRIUMF University of British Columbia, Vancouver, B.C.
  Canada, V6T 2A3

Aluminum dilute alloys oa Al-0.05at.%Cu, Al-0.05at.%Si and Al-0.05at.%Mg were quenched from 600°C or 450°C. The positive muon spin relaxation was measured at Channel M9 of TRIUMF using Arizona (low energy surface) muons. The thickness of the specimens was about 0.4 mm. Sheets of specimens were homogenized at 600°C and quenched from 600°C to the mixture of calcium chloride and water kept at -30°C. The specimens were quickly transferred to liquid nitrogen. The specimens were mounted on the Janis Cryostat without warming up. The muon spin relaxation was measured in these quenched alloy. The depolarization rates of muon spins were measured by zero field method.

For the Al-Cu alloy, the depolarization rate increased from 6 K to 20 K. This corresponds to the increase of the diffusion rate of positive muons as the temperature is raised. It showed a maximum at 20 K and then decreased until 40 K. This decrease corresponds to the detrapping of muons from copper impurity atoms. Then two peaks were observed at 60 K and 90 K. Above 110 K the depolarization rate increased, again correspinding to the increase of diffusion rate of positive muons. After reaching a peak at 200 K the depolarization rate decreased. This corresponds to the mtion of vacancies.

For Al-Si and Al-Mg alloys the general feature is the same as that of Al-Cu, but the corresponding temperatures were different. The largest decrease occurred at about 20 K, 30 K and 60 K for Al-Si, Al-Cu and Al-Mg, respectively. This indicates that the binding energies between a positive muon and an impurity atom are the smallest for the Al-Si alloy, the largest for the Al-Mg alloy among the Al-Si, Al-Cu and Al-Mg alloys. This may indicates that the interaction between impurity atom and a positron may be also important more than we presently understand. Positive muon experiments may clear the interaction between impurity and positrons.

Vacancy -impurity pairs in aluminum start moving at 160 K and 200 K for the Al-Si and Al-Cu alloys, respectively.

THE RECOVERY OF QUENCHED Cu-Ge ALLOYS
STUDIED BY THE POSITRON ANNIHILATION

I.Kanazawa, H.Murakami, T.Kusaka, T.Iwashita and
M.Doyama*

Department of Physics, Faculty of Education, Tokyo Gakugei
University, Nukuikitamachi, Koganeishi, Tokyo 184, Japan.
* Department of Metallurgy and Materials Science, Faculty
of Engineering, The University of Tokyo, Hongo, Bunkyoku,
Tokyo 113, Japan

The recovery of quenched-in vacancies in Cu-Ge alloys
has been studied by the positron annihilation technique.
Specimens, Cu-1.0at%Ge, were prepared by melting Cu and Ge
with 5 nine purity. They were cold rolled and cut into
dimensions of 0.5 mm x 15 mmϕ. ^{22}NaCl droplet of approximately
10µCi was evapolated on a specimen surface and sealed with the
other specimen. They were annealed in Ar atomosphere at
800°C for about 10 hr, and then quenched to methyl alcohol
kept at -90°C. The isochronal and isothermal annealing
treatments were carried out by the methyl alcohol bath
and the oil bath. The methyl alcohol bath and the oil bath
were used in the annealing at temperatures below and above
room temperature, respectively. The temperature of specimen
was kept at -196°C during the measurement of positron
annihilation. The Doppler broadening technique was applied,
and s and h parameters were estimated.
During the isochronal annealing, s parameters decreased
by the annealing from about -30°C to about 20°C, increased
gradually to about 100°C, and then decreased to about 200°C.
The quenching rate in the present study was low since
specimen were thick as 1 mm. Therefore quenched-in vacancies
were trapped by Ge atoms during the quenching. The change
of s parameters below room temperature may show that the
vacancy-Ge atom pair have the rather fast migration rate.
If so, the initial decrease of s parameters are understood as
the annihilation of vacancy-Ge pair at permanent sinks. The
increase of s parameters in the temperature range from 20°C
to 100°C may correspond to formation of small vacancy clusters
and their decrease from 100°C to 200°C may correspond to
dissolution of clusters. The results of isothermal annealing
at 0°C and 150°C support this interpretation. The experiments
and discussions are now progressing in more detail.

A MODEL FOR POSITRON ANNIHILATION IN LIQUID ALLOYS

V.S.Mikhalenkov, V.I.Tokar
Institute of Metal Physics, 252142 Kiev, USSR

A model suggested earlier (I) for positron annihilation in liquid alloys in which positron is considered to be trapped by a vacancy, and the positron-vacancy binding energy is a linear function of the alloy composition in the Ith coordination sphere (c. s.) is extended by taking into account the effects of interatomic interaction.

Introducing the variables $\sigma_i = \pm I$ depending on whether i-position in the neighbourhood of a vacancy is occupied by atom of sort A or B, the energy of system in the regular solution approximation may be expressed in the form

$$E = \frac{1}{4}\omega(c)\sum_{pairs}\sigma_i\sigma_j + \frac{1}{2}\frac{\Delta E_b}{z}\sum_{n.n.}\sigma_i - \mu(c)\sum_i\sigma_i + const.$$

where ω is the mixing energy of liquid binary alloy, ΔE_b is the difference of binding energies between the positron and vacancy for pure A and B metals, z is the coordination number, μ is the chemical potential and c is the concentration of B in A. As in (I) it is supposed that the positron achieves thermodynamical equilibrium in the system before annihilation.

The model calculations were carried out in the mean-field approximation for the system Hg - In with z=8. The concentration dependences obtained for the positron affinity parameter $c\eta$ are shown in Fig. The dotted and solid curves correspond to the assumptions that the alloy composition in the vacancy environment deviates from the average one only in the Ith and in the Ith and 2nd c. s., respectively. ΔE_b value was taken to provide for the best fit with the experimental data of Tsuchiya et al.(2) represented in Fig. by circles. Involving the 2nd c. s. one can obtain non-monotonical concentration dependence of $c\eta$.
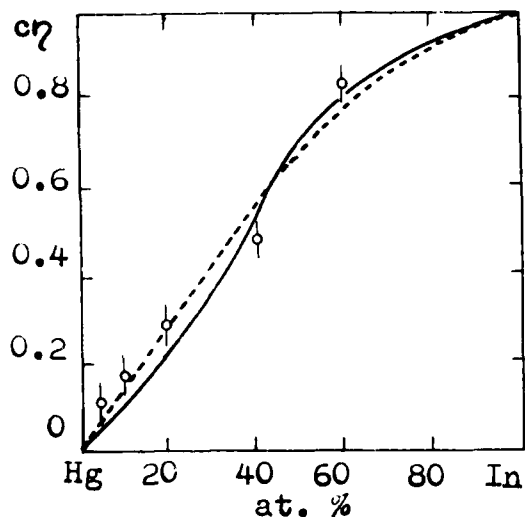
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VACANCY FORMATION ENERGIES IN BCC AND FCC
FeCo BY POSITRON ANNIHILATION

J.A. Jackman, S.M. Kim and W.J.L. Buyers
Atomic Energy of Canada Limited, Chalk River Nuclear Laboratories,
Chalk River, Ontario, K0J 1J0, Canada

A long slit angular correlation apparatus was used to measure the peak coincidence count rate in stoichiometric FeCo from 290 K to 1510 K. The count rate did not change significantly at the order-disorder phase transition (1000 K), but decreased sharply by 3.2% at the bcc-fcc phase transition at 1258 K. The threshold temperatures for thermal generation of vacancies, (T_t), are measured to be 1124 K for the bcc phase and 1260 K for the fcc phase. From the empirical relationship $h^f_v = 15 \, kT_t$, the vacancy formation enthalpies in the bcc and fcc phases are determined to be 1.47 ± 0.05 eV and 1.63 ± 0.05 eV. A constrained trapping model analysis of the bcc phase data, assuming a fixed trapping parameter, yields $h^f_v = 1.51$ eV, in good agreement with the value obtained from the threshold temperature relationship. To our knowledge there is no reliable, direct measurement of the activation energies for self diffusion involving vacancies in this alloy. The activation energies have therefore been estimated from the threshold temperatures, using the empirical correlation of Campbell et al[1], and are found to be 2.45 eV and 2.74 eV for the bcc and fcc phases respectively.

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VACANCY FORMATION ENERGIES IN STAINLESS STEELS
BY POSITRON ANNIHILATION

S.M. Kim and W.J.L. Buyers

Atomic Energy of Canada Limited, Chalk River Nuclear Laboratories,
Chalk River, Ontario, KOJ 1JO, Canada

We have measured the temperature dependence of positron annihilation peak coincidence rate in two bcc stainless steels (Types 430 and 446) and two fcc stainless steels (Types 316 and 310). An S-shaped rise and saturation due to positron trapping at thermal vacancies has been observed in the bcc stainless steels. Trapping model analysis of the data shows that, independent of chromium content, the vacancy formation energy in these alloys is $\approx$ 1.3 eV, close to that in the bcc Fe[1]. For the fcc stainless steels saturation trapping has not been observed up to the melting point. A constrained trapping model analysis of the data shows that the vacancy formation energy in these alloys is $\approx$ 1.6 eV close to that in fcc Fe[1]. Thus the vacancy formation energies in bcc stainless steels are about 20% lower than those in fcc stainless steels. These results indicate that the vacancy formation energies of stainless steels depend more on crystallographic structure than on Cr content.

Vacancy formation energies have been calculated from the known formation energies of iron, nickel and chromium using the theoretical models of Girifalco[2] and Cheng et al.[3] We assumed a bond energy relation v(Fe-Cr) = (v(Fe-Fe) + v(Cr-Cr))/2, that in the fcc phase v(Ni-Ni) = v(Fe-Fe) and that the binding per site for chromium is $\approx$ 20% higher in the fcc phase, as it is for iron. The calculated formation energies were found to be about 10-15% larger than those determined experimentally in the present work.

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POSITRON ANNIHILATION STUDY OF THE VACANCIES IN AgZn ALLOYS

St. Chabik[+] and B. Rozenfeld[++]

[+] Institute of Physics, Pedagogical College, Oleska 48,
45-052 Opole, Poland.

[++] Institute of Experimental Physics, University of Wrocław,
Cybulskiego 36, 50-205 Wrocław, Poland.

Existence of two different positron trapping centers in CuZn
alloys has been reported recently. In [1] they are interpreted as
corresponding to the $\mathcal{L}$ and β phases, whereas in [2] it has sugge-
stet that they corresponds to the different sublatices in ordered
CuZn. The presented here results for   AgZn alloys and especially
for partially ordered monocrystals of the $Ag_{50}Zn_{50}$ alloy, are the
continuation of our former investigations. Mono - and polycrystal-
line samples with different amount of the stable $\mathcal{f}$ and metastable
β' phases have been investigated. The measurements of the tempera-
ture dependence of the peak counting rate $F(T)$ as well as the
x - ray diffraction measurements suggest that in the temperature
interval RT - $270^{\circ}C$ the amount of the $\mathcal{f}$ phase during the heating
run increas at the cost of the β' phase and   above $270^{\circ}C$ the
$\beta' \rightarrow \beta$ and $\mathcal{f} \rightarrow \beta$ phase changes take place. During the cooling
run the $\beta \rightarrow \mathcal{f}$ transition prevails. Assuming the above mentioned
sequence of the phase changes the vacancy formation energies E_v
for the $\mathcal{f}$ (0.5 - 0.6) $\frac{ev}{\sqrt{}}$ and β' (0.4 - 0.5) $\frac{ev}{\sqrt{}}$ phases has been deter-
mined from the $F(T)$ curves by using the trapping model. Similar
values of E_v have been obtained from the so called threshold tem-
perature. The decrease of the vacancy formation energy, E_v, from
1,1 eV to 0.8 eV increasing amount of Zn in the $\mathcal{L}$ phase of the
AgZn alloy has been also confirmed.

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THE INFLUENCE OF THE POSITRON TRAPPING AT VACANCIES ON A PATTERN OF THE FERMI SURFACE OF THE β - BRASS OBTAINED BY POSITRON ANNIHILATION METHOD

B. Rozenfeld[+]   and St. Chabik[++],   J. Pająk[++]

[+] Institute of Experimental Physics, University of Wrocław,
Cybulskiego 36, 50-205 Wrocław, Poland,

[++] Institute of Physics, Pedagogical College, Oleska 48,
45-052 Opole, Poland.

Fermi Surface Anisotropy (FSA) has been investigated for β - phase of the CuZn alloy. FSA has been characterized by the calculated curves of the differences between the experimentally obtained distributions of the free electron momenta for three principial crystallographic directions and averaged distribution calculated by using the Mijnarends method. Angular distribution of the annihilation quanta have been measured conditions permitting the neglection of the trapping of positrons at vacancies as well as for case when almost all the positrons annihilate being trapped at thermal vacancies. It has been found that the FSA measured by means of the positron annihilation technique shows a relatively good agreement with that obtained by dHvA method [1]. However, in the case when the vacancy concentration in the sample exceeds 10^{-5} at% the observation of the directional anisotropy in electron momentum distribution by positron annihilation method is impossible.

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POSITRON TRAPPING IN METAL-METAL AMORPHOUS ALLOYS

E. Cartier, F. Heinrich and M. Küng
Laboratory of Solid State Physics, Swiss Federal Institute of Technology ETH
CH-8093 Zurich, Switzerland

H.-J. Güntherodt
Institut für Physik, Universität Basel
CH-4056 Basel, Switzerland

In recent years a considerable number of positron experiments has been per-formed in transition metal-metalloid amorphous alloys. At the present state of knowledge, it seems to be clear that positrons are trapped at some kind of cavi-ties within these amorphous alloys. The size of such cavities might be non-uniform but seems to be smaller than one atomic volume. Therefore, thermal detrapping might be of significant importance (for details see [1]).

In this contribution we present 2 γ-angular correlation and peakrate measure-ments in various metal-metal amorphous alloys over a wide range of concentrations. The systems investigated are: Cu-Zr, Cu-Ti, Ni-Nb, Ni-Zr, Gd-Co and some simple-metal amorphous alloys.

In crystalline alloys it is well known that positrons can be trapped at clusters of one type of atoms due to different positron affinities to the various components of the alloy. Our results show that besides trapping at small cavities this effect has to be taken into account in amorphous alloys too. In some of the metallic glasses investigated, positrons are trapped at clusters of one of the alloy components. Thermal detrapping from these sites seems to be important and leads to annihilations from a delocalized state in the amorphous matrix at tem-peratures close to the crystallization temperature. By measuring the smearing at the Fermi cutoff it is shown that positrons are delocalized in some simple-metal amorphous alloys.

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THE VACANCY FORMATION ENTHALPY THROUGH THE CU-ZN SYSTEM

P. J. Schultz and I. K. MacKenzie
Department of Physics, University of Guelph
Guelph, Ontario, Canada
N1G 2W1

The dependence of the effective vacancy formation enthalpy
on Zn concentration is followed through both single-phase and
mixed-phase regions for the full phase diagram. No evidence is
found for an appreciable density of structural vacancies in any
of the phases and there is remarkably little evidence of
sensitivity to the order-disorder transition in the β phase
from lineshape measurements; lifetime data show a very small
but significant change at the order-disorder transition.

POSITRON ANNIHILATION IN B2-ORDERED TRANSITION METAL ALLOYS

M. Šob

Institute of Physical Metallurgy, Czechoslovak Academy
of Sciences, Žižkova 22, 616 62 Brno, Czechoslovakia

Common features of the electronic structures of B2-orde-
red stoichiometric transition metal alloys and their manifesta-
tions in the momentum densities of annihilation photons are
discussed. It is shown that the low-energy parts of band struc-
tures have the same character in alloys AB, where A is a 3d-me-
tal and B is another 3d-metal or a simple metal with lower ato-
mic number than A, and are similar to the corresponding parts
of band structures of 3d-metals with the bcc lattice considered
as the CsCl-type lattice with identical atoms. Except for the
lowest band, the states belonging to these bands are determined
primarily by the 3d-states of the metal A. The band-structure
calculations and the analysis of the electron distribution in
alloys FeAl and FeTi illustrate quantitatively these conclusions
which serve as a basis for a discussion of the differences
between the momentum densities of annihilation photons in the
B2-ordered transition metal alloys.

INVESTIGATION OF THE ELECTRONIC STRUCTURE
OF Fe-Co ALLOYS BY POSITRON ANNIHILATION AND THE
MÖSSBAUER EFFECT

J.Chojcan, M.Szuszkiewicz, S.Szuszkiewicz, B.Rozenfeld
Institute of Experimental Physics, Wrocław University,
Cybulskiego 36, 50-205 Wrocław, Poland

The angular distributions of annihilation quanta coming from two-photon annihilation of an electron-positron pair as well as the Mössbauer spectra of ^{57}Fe have been measured for polycrystalline samples of Fe and bcc Fe-Co alloys. On the basis of these measurements, the authors are going to estimate the distributions of 3d-like electrons in the Fe-Co alloys and to get some information about the direction of the electron transfer between the alloy components.

ANGULAR CORRELATION MEASUREMENTS ON Nb-Mo SYSTEM

N. Shiotani, T. Okada, H. Sekizawa and T. Nakamichi*
The Institute of Physical and Chemical Research,
Wako-shi, Saitama 351, Japan
*The Research Institute for Iron, Steel and Other Metals,
Tohoku University, Katahira, Sendai 980, Japan

Niobium and molybdenum have nearly the same electronic band structure, especially at and below the Fermi level. The Fermi level is higher in Mo than Nb because of the extra valence electron per atom. Consequently, measurements of the angular correlation of annihilation radiation in a series of binary Nb-Mo alloys should provide information on how the addition of d electrons to the unfilled d band changes the geometry of the Fermi surfaces. The Nb-Mo system forms a complete series of disordered solid solutions all having a body-centered cubic structure, thus permitting intercomparisons to be readily made. Preliminary but quite important results of 2D angular correlation measurements were reported on Nb, $Nb_{90}Mo_{10}$, $Nb_{70}Mo_{30}$ and Mo by West[1]. Calculations of the band structure of this system were reported by Colavita et al[2] based on the CPA scheme and by Nakao and Wakoh[3] based on the ATA scheme.

We measured one dimensional angular correlation curves of Nb, $Nb_{80}Mo_{20}$ and $Nb_{50}Mo_{50}$ by a parallel slit system. The angular resolution of the system is 0.60 mrad. The single crystals were grown by zone melting in an argon arc furnace. The experimental results are shown in Fig. 1. The experimental curves will be compared with theoretical ones obtained from the rigid band model for $Nb_{80}Mo_{20}$ and those obtained from the ATA calculations by Nakao and Wakoh for $Nb_{50}Mo_{50}$.

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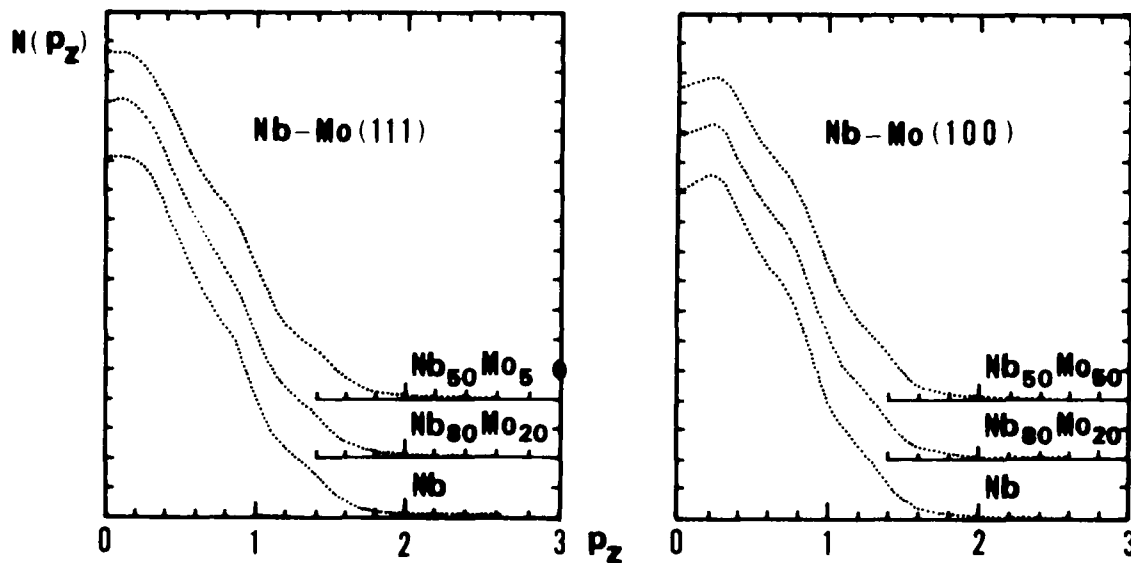[3] Y. Nakao and S. Wakoh, J. Phys. Soc. Jpn. 49, 2423 (1980).

Fig. 1. Angular correlation curves $N(p_z)$, p_z is in atomic units.

POSITRON ANNIHILATION ON LOW DIMENSIONAL CONDUCTORS
(the metallic-polymer (SN)x)

Y. Suzuki, I. Suzuki, S. Matsusaki, M. Doyama, I. Nakada[**]
Department of Metallugy and Materials Science, Faculty of Engineering,
The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo, Japan
**The Institute for Solid State Physics, The University of Tokyo,
7-22-1 Roppongi, Minato-ku, Tokyo, Japan

Doppler broadening and life-time studies of positron annihilation for (SN)x have been made. The energy bands of (SN)x refered quasi-one-dimensional metallic chractristics, have different structure from metals.

The unit cell of (SN)x is monoclinic system (space group $P2_1/C$) and many band-structure calculation have been made. The results, however, are different from one another.

The band calculation by Oshiyama[1] using self-consistent numerical-basis-set LCAO method, shows that bands split in four different bands. Fig 1. shows the outer surfaces. They close in Kb directions (main chain directions) and connected in Ka and Kc directions.

We measured the Doppler broadening in three directions around Ka, Kb and Kc. (Its axis shifted 20 degrees from right angle.)

The results of Doppler broadening using H-parameters, show its character-istics of broadening Ka, Kb and Kc. In the direction around Ka, the data of H-parameter have peaks at the direction for Kb, but the B. Z. width for Kc is narrower than that for Kb. The difference of H-parameter around Ka or Kc, between maximum and minimum is 0.005. The one for Kb direction is 0.002. This is less than other two directions. That means free electrons for Kb (main chain directions) are many and condenced. The results supported Oshi-yama's band calculation.

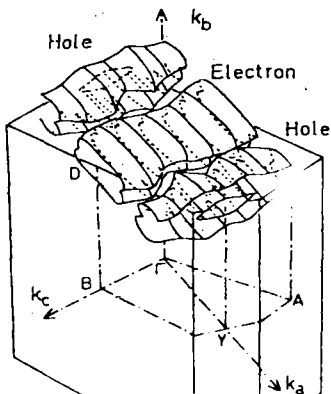1) A Oshiyama private communication.

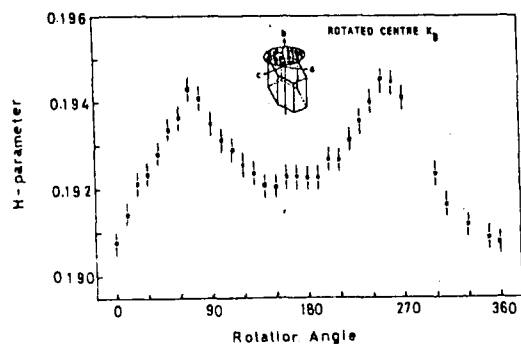

Fig 1. The band calculation by Oshiyama.[1]

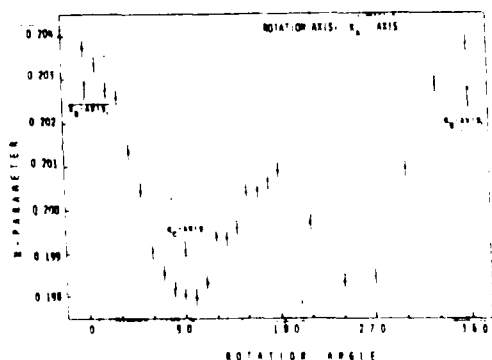Fig 2-1 H-parameter in Doppler broadening around Kb axis
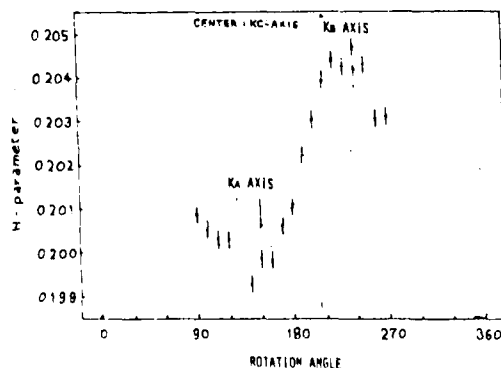

Fig 2-2 Around Ka axis

Fig 2-3 Around Kc axis

MOMENTUM DENSITY MEASUREMENTS IN COPPER
BY ANNIHILATION RADIATION*

F. Sinclair, W. S. Farmer, and S. Berko
Physics Department, Brandeis University
Waltham, Massachusetts 02254, U.S.A.

A high precision reconstruction of $\rho(\underline{p})$ in three dimensions for copper has been calculated using two dimensional angular correlation of annihilation radiation (2D ACAR) data. The cross-coincidences from two banks of 32 scintillation detectors[1] with circular collimation 0.75 mrad in diameter were recorded for 15 different integration directions separated by 9° in the (100) and (110) planes. This enables the reconstruction of $\rho(\underline{p})$ in planes normal to [100] and [110] separated by 3.6 mrad. A 0.2 mrad mesh was used within the planes, where the resolution was ~0.8 mrad radially and circumferentially except beyond ~5 mrad from the center, where the 9° interval between projections results in a worsening circumferentially.

The reconstructed $\rho(\underline{p})$ shows the Fermi surface quite clearly, in close agreement with the analytical parametrization due to Halse. The Umklapp annihilations are clearly observed in the second zone of both independent planes of data.

Comparison of the reconstructed $\rho(\underline{p})$ with two independent-particle-model (IPM) calculations[2,3] shows clearly a momentum-dependent many-body enhancement that increases the annihilation rate as $|p| \to |p_f|$.

By carrying out a circular average of our data for $|p| \leqslant 4$ mrad and comparing our results to the IPM calculations, we have parametrized the enhancement using Kahana's[4] formulation, yielding $b/a = .131 \pm .020$ and $c/a = .110 \pm .036$. These results are in reasonable agreement with theoretical predictions.[5]

We have also compared our data to the results of an empirical reformulation of the enhancement in terms the energy rather than momentum,[3] leading to quite close agreement.

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CALCULATION OF POINT SLIT ANGULAR CORRELATION CURVES IN PARAMAGNETIC CHROMIUM

A.K. Singh and R.M. Singru
Department of Physics, Indian Institute of Technology,
Kanpur, 208 016, India.

Measurement of the point slit or two-dimensional angular correlation of positron annihilation radiation (2D-ACPAR) is of special interest in studying the Fermi surface and momentum distributions of transition metals as shown by the results on Cu[1] and V.[2] In our program to calculate the 2D-ACPAR curves using band wave functions we have chosen chromium (Cr) because i) it is next to vanadium and thus provides an interesting comparison ii) it has a complicated FS and iii) it has an interesting magnetic structure (involving spin density waves) at $T < 312$ K which can be partly understood from the FS of nonmagnetic Cr.

Chromium has partially filled 3d states and this gives rise to four sheets of FS in the paramagnetic phase ($T > 312$ K): i) electron surface (jack) around Γ, ii) electron pockets (lenses) centered on the Δ symmetry axes, iii) octahedral hole surfaces centered around H and iv) ellipsoidal hole pockets centered around N. Measurement of the 2D-ACPAR curves, $N(p_y, p_z)$, along different sets of directions in Cr can, therefore, provide us with valuable information about the FS of Cr. In order to compare such measured data with theory and to examine the band structure effects on $N(p_y, p_z)$ it is necessary to perform a band structure calculation of $N(p_y, p_z)$. Previously such calculation for the long slit or 1D-ACPAR curves, $N(p_z)$, have provided an interesting comparison with experiments.[3] We report here a band structure calculation of the $N(p_y, p_z)$ curves for paramagnetic Cr.

The starting point of our calculation was the self-consistent crystal potential for non-magnetic Cr prepared by Wakoh and reported by Asano and Yamashita.[4] The band structure and two-photon momentum distributions were calculated using the fast approximation scheme of Hubbard as modified by Mijnarends.[5] Other details of the calculation are described in the earlier report on Cu.[1] Our results for the energy bandwidths as well as that for FS topology show a good agreement with other theoretical and experimental results. The 2D-ACPAR curves $N(p_y, p_z)$ calculated for different sets of orientations will be presented and the results discussed in terms of partial contributions from different bands and FS topology. These results are interpreted to show which parts of the FS can be examined in each orientation. The present results of $N(p_y, p_z)$ for Cr are compared with those calculated for V[2] and the differences are analysed in terms of their band structure and FS. Similarly a comparison of the results for Cr and VD$_x$[2] is made to bring out the limitations of the rigid band approximation.

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THE RECONSTRUCTION OF THE TOTAL MOMENTUM DISTRIBUTION
FROM TWO - DIMENSIONAL ACPAQ EXPERIMENTAL RESULTS

G. Kontrym - Sznajd
Institute for Low Temperature and Structure Research,
Polish Academy of Sciences,
Pl. Katedralny 1, 50-950 Wrocław, Poland.

The methods of determining the total electron-positron momentum distribution $\rho(p)$ by positron annihilation are discussed for crystals with a given symmetry[1,2,3]. Application of Cormack's method to two-dimensional ACPAQ (angular correlation of positron annihilation quanta) model curves is presented for hcp structure. A method for describing higher momentum components is proposed in order to reconstruct $\rho(\underline{p})$ better. The results obtained for some models of $\rho(\underline{p})$ are good showing that the method works well.

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THE FERMI SURFACE OF GADOLINIUM

R. L. Waspe and R. N. West
School of Mathematics and Physics
University of East Anglia, Norwich, England

The Fermi surface of hexagonal Gadolinium is highly structured and anisotropic and, as a consequence, so also is the electron momentum density. Sixteen different high precision 2-d angular distributions for Gd have been obtained by progressive rotation of a single crystal through 2° intervals throughout a symmetry element of the basal plane lattice. These distributions have been used as the input for a reconstruction of the 3-d distribution in k-space which employs the LCW folding[2] and tomographic reconstruction techniques. The results are compared with contemporary pictures of the Fermi surface of Gd.

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TWO-DIMENSIONAL ANGULAR CORRELATION STUDIES
OF TRANSITION METALS AND ALLOYS

J. H. Kaiser, P. A. Walters, R. L. Waspe and R. N. West
School of Mathematics and Physics
University of East Anglia, Norwich, England.

A large number of studies of transition metals and alloys have now been performed on the UEA 2-d machine[1]. Analyses of the measured momentum space densities and the related k-space densities obtained by the LCW folding procedure[2] has yielded a wealth of detail concerning the underlying electronic structures. Among the matters discussed in this paper are the essential features of the Fermi surfaces of Y, V, Cr, Nb and Mo, the developements accompanying alloying of Nb with Mo, and the effects of magnetic ordering in Cr. In each case the results are discussed in the light of relevant band structure calculations.

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STRUCTURAL CHANGES IN $(Mo_{.6}Ru_{.4})_xB_{1-x}$ AMORPHOUS ALLOYS STUDIED WITH POSITRON ANNIHILATION

R. H. Howell
Lawerence Livermore National Laboratory
Livermore, California 94550
and
W. L. Johnston
California Institute of Technology
Pasadena, California 91125

Changes in the structure of amorphous alloys of $(Mo_{.6}Ru_{.4})_xB_{1-x}$ introduced by irradiation or by varying the boron fraction were studied by both positron lifetime and Doppler broadening measurements. The alloy with a boron fraction of 18 percent is expected to contain the least free volume, all open volume being occupied by boron atoms. This alloy produced the lowest lifetime and also the lowest Doppler broadening peak parameter. Small increases in the lifetime and Doppler broadening peak parameter were observed for both those samples with a smaller than optimal boron fraction (13 percent) and the 18 percent boron fraction samples which were irradiated by neutrons. In the 13 percent boron samples an average of the annihilation rates of the individual constituents would lead to a shorter lifetime than the 18 percent alloy. An increase in the positron annihilation parameters indicates that more open volume is available in those samples. Both the irradiated and the low boron fraction samples can be described as containing open volume regions which interact with the positron similar to the positron-defect interaction seen in crystaline materials. These results are consistent with those obtained from small angle x-ray scattering from the same samples.

POSITRON ANNIHILATION STUDIES OF AMORPHOUS ALLOYS

Mbungu Tsumbu (*), D.Segers (*), L.Dorikens-Vanpraet (*),
M.Dorikens (*) and K.H.J.Buschow (**)

(*) I.N.W., Proeftuinstraat 86, B-9000 Gent, Belgium
(**)Philips Research Laboratories, 5600 MD Eindhoven,
    The Netherlands

The crystallization behaviour of amorphous alloys was studied with the positron annihilation technique and also with X-ray diffraction measurements. Lifetime and Dopplerbroadening studies were carried out on the amorphous alloys Metglas 2826MB [i.e. $Fe(40)Ni(38)Mo(4)B(18)$], Metglas 2605SC [i.e. $Fe(81)B(13.5)Si(3.5)C(2)$] and $Zr(70)Ni(30)$, as a function of temperature. From the positron annihilation measurements it was concluded that the Bernal dense random packing model gives a valid description for the structure of the alloys in the amorphous phase. The trapping behaviour of the positrons in the amorphous alloys is briefly discussed.

POSITRON ANNIHILATION STUDY IN THE RECOVERY PROCESS
OF AMORPHOUS $Fe_{40}Ni_{40}P_{14}B_6$ ALLOY

Masao Doyama, Takashi Mihara[*][#] Shuichi Otake[*] and Hiroshi Fukushima

Department of Metallurgy and Materials Science
Faculty of Engineering, The University of Tokyo
7-3-1 Hongo, Bunkyo-ku, Tokyo 113 Japan

* Department of Physics, Faculty of Science, Science University of Tokyo
Kagurazaka, Shinjuku-ku Tokyo 162 Japan

Positron annihilation behavior is quite sensitive to vacancy type lattice defects. Amorphous alloys contain a large number of lattice defects. Therefore, the positron study in the amorphous state may be one of the quite sensitive techniques to study small changes occured in the structural changes in the amorphous state.

The specimen used in the present experiment was amorphous $Fe_{40}Ni_{40}P_{14}B_6$ alloy (Metglas 2826, a commercial product by Applied Chemical Co.) produced by rapid quenching. The isochronal annealing (15 min) was performed. The Doppler broadening profile of 511 KeV annihilation line was studied. Positron lifetime and electrical resistance were also measured.

In the isochronal annealing, W parameter started increase at about 470 K and 590 K. Those two peaks took place below crystallization temperature. Since a positron is trapped or stay longer time at an excess free volume or larger Bernal holes, the annihilation rate with core electrons is increased by the loss of excess free volume.

W parameter changes in isothermal annealing at 523 K follows the relation

$$W(t) = W_q + \Delta W (1 - \exp(-t/\tau))$$

where the values of W_q, ΔW and τ were determined to be 0.2555 ± 0.0004, 0.0015 and 10 minutes, respectively.

The positron lifetime was best represented by one component other than source component. This indicates that all positrons are weakly localized at the space between the metal ions (Bernal holes). After annealing at 530 K in isochronal annealing. Slight increase by annealing was observed. The changes measured at 77 K and 300 K were not proportional. This indicates that the electrical resistivity in this alloy does not obey Methiesen's rule. The vibrational modes changed as the annealing proceeds.

Near 420 K quenched excess volume probably large Bernal Holes anneal out. This migration causes the short range migration of the constituent atoms and the short range order is changed. This is probably the reason of increase of electrical resistivity. Length is reported to contract in this stage. The change near 600 K in positron annihilation behavior is probably due to the diffusion of alloying elements. The diffusion of alloying elements in the amorphous state may not require the assistance of vacancies. Atoms are pushed from compression region to expanded region, one atom by one or as a string of atoms. The displacement of an atom in the elementary diffusion process could be shorter than the nearest neighbor distance.

Present address: Hitachi Micro-computer Engineering Co. 1479 Kamimizu-
honmachi, Kodairashi Tokyo 187 Japan

POSITRON ANNIHILATION IN VARIOUS TYPES OF GLASSY METALS

S. Tanigawa[#], K. Shima[#], H. Iriyama[#] and Y. Waseda[##]

#) Institute of Materials Science, University of Tsukuba,
Sakura-mura, Ibaraki 305, Japan

##) Research Institute of Mineral Dressing and Metallurgy,
Tohoku University, Sendai 980, Japan

In the early stage of application of positron techniques to glassy metals, it has been misunderstood that glassy state contains no trapping centers for positrons, due to the small changes in positron parameters upon crystallization. Recently, however, the precise measurements of positron lifetimes, Doppler broadening of annihilation lines and so on revealed the abundant presence of trapping centers both in glassy and crystallized states. In the present paper, measurements of positron lifetimes, Doppler broadening and the two parameter correlation of positron age-momentum were applied to various types of glassy metals, i.e., $Pd_{80}Si_{20}$, $Co_{73}Fe_5Si_{12}B_{10}$, $Fe_{80}B_{20}$, $Fe_{40}Ni_{40}B_{20}$, $Fe_{40}Ni_{40}P_{14}B_6$, $Cu_{35}Zr_{65}$, $Cu_{50}Zr_{50}$, $Cu_{65}Zr_{35}$ and $Ni_{90}Zr_{10}$ alloys. In Figs. 1 and 2, the isochronal annealing curves of lifetimes in $Pd_{80}Si_{20}$ and $Co_{73}Fe_5Si_{12}B_{10}$ are shown. The behabior of these two alloys is very similar. This means the importance of Bernal holes before crystallization and of grain boundaries after crystallization as trapping centers for positrons. Figure 3 shows the isochronal annealing results in $Fe_{40}Ni_{40}P_{14}B_6$. The value of lifetime in as-quenched state is longer than deformed iron. Figure 4 shows the difference of Doppler broadening profiles in glassy Cu-Zr system relative to that in well annealed copper. It was found that positrons annihilate at sites of similar circumstance to those in well annealed zirconium.

Figure 5 shows the resolved lifetime as a function of Doppler broadened energy channel in $Co_{73}Fe_5Si_{12}B_{10}$. The clear dependence of lifetime on momenta means the coexistence of several annihilation modes and predicts the size distribution of Bernal holes.
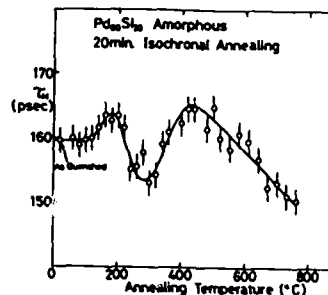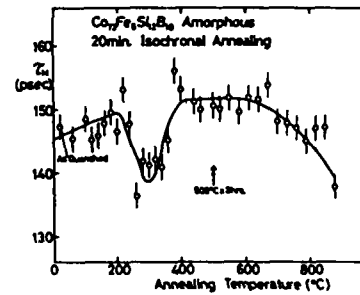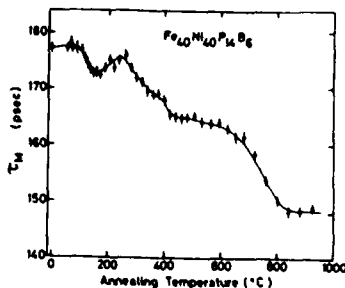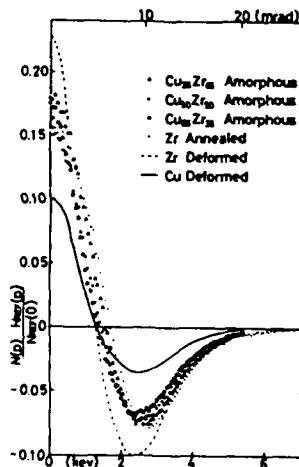

Fig. 1

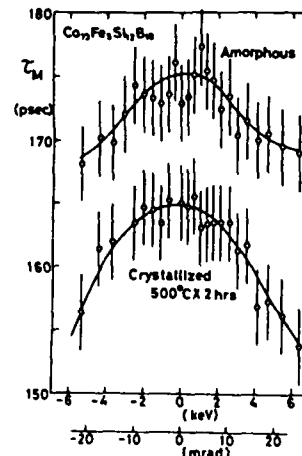
Fig. 2

Fig. 3

Fig. 4

Fig. 5

TEMPERATURE DEPENDENCE OF THE POSITRON DIFFUSION LENGTH IN METALLIC GLASSES AS STUDIED BY VARIABLE-ENERGY POSITRONS

K. G. Lynn, A. Vehanen, P. J. Schultz, A. N. Goland, C. L. Snead, Jr.
Brookhaven National Laboratory*
Upton, New York 11973, U.S.A.

H. J. Güntherodt
Institut für Physik
Universität Basel
CH-4056 Basel, Switzerland

E. Cartier
Laboratorium für Festkörperphysik ETH
Eidgenössische Technische Hochschule
CH-4056 Zürich, Switzerland

The first studies showing the temperature dependence of the positron diffusion length as examined by slow positrons will be presented for four different metallic glass systems (i.e. $Cu_{30}Zr_{70}$, $Cu_{50}Zr_{50}$, $Fe_{82}B_{12}Si_6$, and $Fe_{40}Ni_{40}P_{14}B_6$). All of the samples exhibited a short diffusion length in the as-received condition consistent with a large concentration of positron trapping centers. The concentration of these trapping sites varies from sample to sample but the data indicate that positrons are trapped in these metallic glass samples at 300K. The positron diffusion length did not significantly increase until temperatures well above the usually reported crystallization temperature. This is interpreted as evidence that the samples still have a large concentration of trapping centers after crystallization (possibly dislocations or grain boundaries). When the samples were fully crystallized and annealed we found increases in positron diffusion lengths in some cases by as much as two orders of magnitude, with the final value being consistent with a defect-free metal. Standard Doppler-broadening measurements were also performed simultaneously on the $Cu_{50}Zr_{50}$ sample and correlations between the specific changes of the S parameter and the diffusion length will be discussed.

DOPPLER BROADENING MEASUREMENTS ON STABLE METALLIC GLASSES AT TEMPERATURES NEAR T_g

S. Y. Chuang

Center for Positron Studies, The University of Texas at Arlington,
Arlington, TX 76019, USA

H. S. Chen

Bell Laboratories, Murray Hill, NJ 07974, USA

Doppler boroadening measurements have been made on two metallic glasses, $Pd_{.77}Cu_{.06}Si_{.165}$ and $(Pt_{.8}Ni_{.2})P_{27}$, at temperatures from room temperature up to crystallization temperature of the samples. Correlation between the line-shape parameter (S) of the Doppler spectrum and the glass transition temperature T_g will be presented.

POSITRONIUM FORMATION IN HELIUM

D.R. Cook, P.G. Coleman, L.M. Diana, S.C. Sharma
Center for Positron Studies, Box 19059, UTA Station
The University of Texas at Arlington, Arlington, Texas 76019, U.S.A.

A study of the positronium formation cross section for positron-helium collisions is in progress. The experimental method exploits the fact that positronium formation is the only scattering channel which essentially neutralizes the positron and renders it undetectable. By constraining all the other positrons, scattered or unscattered, to paths ending at a detector, one can measure directly the fraction f of the incident beam which is removed by positronium formation. The method relies, then, on detecting those positrons which do not form positronium, rather than detecting the positronium formed[1].

If the total cross section Q_{tot}, and the gas density-path length product nx, are known, then the positronium formation cross section Q_{Ps} is simply given by

$$Q_{Ps} = \frac{f}{(1 - \exp(-nQx))} \, Q_{tot}.$$

In the experimental apparatus a beam of monoenergetic positrons of controllable energy pass through a gas cell to a channel electron multiplier (CEM). The beam is produced by bombarding an annealed tungsten mesh with beta positrons from 100 microcuries ^{22}Na. The flight tube is surrounded by a solenoid which produces a uniform, axial, 200G magnetic field. When helium is introduced into the cell at a density at which 10-15% of the positrons undergo collisions, the scattered and unscattered positrons are constrained by the field to reach the CEM detector. Positrons scattered into the backward hemisphere are reflected at the source and pass through the cell again on their way to the detector. The CEM count rate is recorded with and without gas in the cell, and background rates are subtracted in both cases. The background rate is reduced by removing any CEM pulses which are coincident with pulses from a thin scintillator which covers the ^{22}Na source. These pulses are due to fast (unmoderated) positrons from the source.

The main source of error in this method stems from the possiblity of forming positronium in a second or third collision. Generally in these measurements an inelastic collision will throw the positron down to energies below the positronium threshold, but Ps formation may follow elastic scattering and corrections (expected to be no more than 10-15%) must be applied to allow for this when calculating absolute Q_{Ps} values.

Preliminary results of the measurements will be presented at the meeting.

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DIFFUSION OF POSITRONS IN NOBLE GASES AT HIGH FREQUENCIES

P.S. Grover
Department of Physics & Astrophysics
University of Delhi, Delhi, India.

Annihilation decay rates for positrons in noble gases
helium, neon and argon have been determined in the presence of
external steady magnetic field and high frequency varying
electric fields. The decay rates depend quite sensitively on
the strength of the fields and the frequency of the electric
field. They show a minima when the frequency of the electric
field equals the cyclotron frequency. The effect is maximum
in helium and decreases as the atomic weight of the gas
increases.

The sensitivity of the results to the positron-atom
interaction model has also been studied.

ON THE POSITRON ANNIHILATION IN HELIUM

P.S.Grover

Department of Physics, University
of Delhi, Delhi-110007, India.

Numerical calculations of the average energy and
annihilation rate of positrons in helium gas have been
made over a wide range of electric (0 - 50 Vcm^{-1}) and
magnetic (0 - 1oo kG) fields at various temperatures.
Two models of positron-atom interaction have been consi-
dered. Our computations indicate that the positron
energy and life time decrease with the magnetic field,
at given electric/temperature fields. When the electric
field is zero, magnetic field has no effect on the
above parameters. This observation is in agreement with
the recent experiments of Canter [1].

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MODEL POSITRON-ELECTRON CORRELATION POTENTIAL FOR POSITRON BOUND-ATOMS AND ANIONS

S. W. Chiu and D. M. Schrader
Department of Chemistry
Marquette University
Milwaukee, WI 53233, U.S.A.

An SCF theory for one-positron many electron systems[1] provides the correct correlation behavior for all positron-electron Pairs; however, it has proven difficult to apply in calculations. The essential features of this theory are preserved and the applications simplified by modelling the dynamical screening of the electron-positron interaction with an effective correlation potential of the Yukawa type. The representation of the dynamical screening effects reduces to the selection of an effective screening function, β. By an iterative technique, vestiges of β in the wave function can be successively reduced, but at every step in the iteration process a variational bound on the energy is available.

In our work we deduce a suitable functional form for β which permits the accurate calculation of positron scattering cross sections or binding energies and positron annihilation characters for atomic systems. To carry out the calculation, we are adapting the BISON SCF program for diatomic molecules[2]. Test results on positron-atomic hydrogen scattering will be presented.

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ANGULAR CORRELATION OF TWO-PHOTON PAIR ANNIHILATION
RADIATION FOR POSITRONS ANNIHILATING IN NITROGEN

J.W. Darewych
Physics Department
York University, Toronto, Canada M3J 1P3

The angular correlation of two-photon pair annihilation radiation for positrons annihilating in gaseous N_2 is calculated at zero energy. The $e^+ - N_2$ wave function is obtained from a model in which the interaction between the positron and the N_2 is described as a superpositron of a static plus cut-off polarization potential, where the cut-off parameter is adjusted so that the calculated elastic cross section at low energy agrees with observed results. The present calculations are compared to experimental measurements of the angular correlation in liquid nitrogen.

SIMPLE, VARIATIONALLY OPTIMIZED WAVE FUNCTIONS
FOR LOW ENERGY e^+ - H SCATTERING AND ANNIHILATION

J.W. Darewych, R.P. McEachran and M. Horbatsch
Physics Department
York University, Toronto, Canada M3J 1P3

We calculate the elastic s-wave scattering phase shifts $\eta(k)$ and effective number of annihilation electrons Z_{eff} for incident positrons in the momentum range $0 \le ka_0 \le 0.8$, using a trial wave function of the form

$$\Psi_T = F(x)\psi_0(r) + \phi(x)\psi(r)P(s),$$

where x,r, and s are the e^+-P, e^--P and e^+-e^- distances respectively. $\psi_0(r)$ is the H ground state wave function, while F, ϕ, ψ, P are determined from the variational principle $\langle \delta\Psi_T|\hat{H} - E|\psi_T\rangle = 0$. Here $\hat{H}$ is the hamiltonian and E the total energy of the system. The variational functions are subject to $F(x\to\infty) = \sin(kx + \eta)/kx$ and the closed channel part $\phi\psi P$ being square integrable. We consider initially restricted variations in which: (1) F and ϕ are allowed to vary freely but ψ and P are taken to be simple analytic forms, $e^{-\beta r}$ and $e^{-\gamma s}$ respectively; (2) F, ϕ, ψ are allowed to vary freely but $P = e^{-\gamma s}$. The parameters γ (and β) are chosen to maximize η (which is a lower bound on the exact phase shift). In the case of (1) we discuss the effect of the monopole correction

$$P(s) \to P(s) - \frac{\sinh\gamma r}{\gamma r} e^{-\gamma x}.$$

The resulting, variationally optimized, trial wave functions are used to calculate $Z_{eff}(k)$. A comparison with other calculations is given.

INELASTIC SCATTERING OF POSITRONS BY HE ATOMS

R.P. McEachran, L.A. Parcell[†], A.D. Stauffer
York University, Downsview, Ontario
Canada, M3J 1P3

The cross section for excitation of the helium atom to the 2'S state by collisions with positrons is calculated using a distorted wave approximation. The distorting potentials in each channel are the sum of the respective static and polarization potentials. The polarization potential for the ground state is taken from a polarized orbital calculation[1], and this potential, scaled to have a dipole polarizability equal to that of the excited state[2] is used as the polarization potential for the excited state. The calculated differential and total cross-sections are compared with recent experimental results[3] for excitation of the 2'S state within 10eV of threshold.

[†]permanent address: School of Mathematics and Physics, Marquarie University,
North Ryde, NSW 2113 Australia

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DIAGNOSTICS OF PLASMA BY THE METHOD OF POSITRON LIFE-TIME

Arifov P.U.,   Shevchenko A.V.,   Shevelev S.V;

Arifov's Institute for Electronics,   Tashkent,   USSR

It was showed in workes /I,2/ that it is possible to get the information on temperature T_- and concentration n_- of electrons in plasma according to experimental spectra of angular correlation of annigilation quanta.Present work analyzed possible ways of n_- determination of light elements plasma from the observed time spectra of positron annihilation.

When $n_+ \ll n_-$ than spectrum of positron annihilation, being the initial moment of time t=0 in plasma, is as follows

$$I(t) = I(0) \exp(-t/\tau_a)$$

where $I(t)$, $I(0)$ are rate of annihilation at the moment t and at the initial moment,respectivly; τ_a is the time of life thermalized positrons with reference to 2γ-annihilation,depending from n_- and T_-/2/. Using measurement data $I(t)$,$I(0)$ it is possible to find τ_a value.The use of Ge(Li) detector allows to registrate energetic spectra of γ-quanta and thus to obtain the information on the T_-. If we know the T_- and τ_a it is possible to determine n_- from the equation for τ_a /2/. As opposed to the method described /2/ doesn't require the information on positron concentration n_+ as in this case positron concentration doesn't effect τ_a value.

Performing of the mentioned technique is connected with the fulfilment of $\tau_o \ll \tau_a$ condition (τ_a is the time of thermalizathon of hot positrons,injected into plasma) and with possibility of $I(t)$ value provision wich is necessary for accumulation of sufficiently extensive statistics of N for the time of plasma existance.In /I/ there evaluated the time τ_o for positrons,injected in plasma along the lines of magnetic field pronided thah they are thermalized up to temperature $T_+(\tau_o)-T_-=0.1T_-$ (T_-=10 and 100 eV). For positrons with energies of > 10 keV the probability of escape without annihilation from plasma trap with the size 1 m is very high throughout the whole range of the n_-: $10^{12}-10^{17}$ sm^{-3}. Consequently, it's better to use positrons with energies < 10 keV as it would simultaneously provide the fulfilment of $\tau_o \ll \tau_a$ condition.

The positron injection rate into substance,determining $I(t)$ and the time of N accumulation, limited by $\leq 1/\tau_a$ value.The application of conventional technique for plasma under consideration, in wich τ_a makes up fraction and units of seconds,leads to the abrupt increase in time of N accumulation in comparisen,for instance,to solids,where $\tau_a \simeq 10^{-7}-10^{-10}$ sec.Tnis fact doesn't allow to use the conventional technique for plasma investigation in device with pulse effect or for the study of dinamic process.

To overcome this difficulty we propose to unject simultaneously sufficient number of positrons into plasma during the time much less than τ_a.In this case $I(t)$ will be restricted by resolution time of registrating instruments ($\tau \approx 10^{-7}-10^{-9}$ sec) and as $\tau \ll \tau_a$ the time of statistics accumulation can be decreased by increasing of initial concentration $n_+(0)$.The evaluation showes that $n_+(0)=10^3-10^4$ sm^{-3} is sufficient for plasma under consideration.Such positron concentration can be obtained with the help of instruments /I/,wich operate within pulse regime.

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LINESHAPE EFFECTS IN THE MEASUREMENT OF
THE POSITRONIUM HYPERFINE INTERVAL

Allen Mills, Jr.
Bell Laboratories, Murray Hill, NJ 07974 USA

Recently Rich[1] has pointed out that annihilation terms in the effective 4x4 Hamiltonian H for n=1 positronium cause the real parts of the Zeeman eigenvalues to be shifted by terms of order $(\lambda_s/4\pi\Delta\nu)^2 \sim 10^{-5}$ relative to the Breit-Rabi eigenvalues. Here λ_s is the annihilation rate of the singlet state and $\Delta\nu$ is the hyperfine interval. Rich observes that the $\Delta\nu$ measurements have not correctly dealt with decay. The Zeeman resonance lineshape is calculated here assuming that the non-Hermitian H describes the motion of the four n=2 levels via Schroedinger's equation.[2] The deviations of this lineshape from a Lorentzian are exhibited. The asymmetry of the line causes a shift in the line center relative to what one would obtain from a Breit-Rabi plus Lorentzian fit to a measured Zeeman resonance curve. To take this into account, the 1975 Brandeis measurement[3] of $\Delta\nu$ should be increased by 2.5 ppm to $\Delta\nu$(Brandeis)= 203.3875(16) GHz. When the 1975 Yale measurement[4], which used a different lineshape, is reinterpreted in terms of the lineshape calculated here, the Yale $\Delta\nu$ value increases by 21 ppm to $\Delta\nu$(Yale) = 203.3890(12) GHz. The weighted mean of the two corrected measurements is $\Delta\nu$=203.3885(10) GHz.

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A PRECISE MEASUREMENT OF THE POSITRONIUM HYPERFINE INTERVAL

M. W. Ritter et al.
Physics Department, Yale University,
217 Prospect Street, New Haven,Conn. 06511, U.S.A.

INTERACTIONS OF POSITRONS WITH CHARGED ATOMIC AND MOLECULAR SPECIES

A. Barry Kunz
Physics Department
Michigan Technological University
Houghton, Michigan 49931

and

James T. Waber
Department of Materials Science and Engineering
Northwestern University
Evanston, Illinois 60201

Evidence is presented that a positron will not bind at a positively charged or at a neutral molecule if it possesses high point group symmetry. Two isoelectronic sequences, Ne^+, F and OH as well as Ne, F^- and OH^- have been studied. In addition, the neutral molecules, HF, H_2O, NH_3 and CH_4 and the solvated electron H_2O^- have been investigated.

Large basis sets with very diffuse electronic orbitals are necessary for those systems which do bind a positron in order to converge the total energy to the Hartree Fock limit.

Correlation plays a very significant role in very loosely bound systems A Second Order Many Body formulation has been used to calculate the binding energy in molecular positron systems.

The force calculated from the Gradient of the total energy between a positron and several atoms in the molecules has also been studied.

QUANTUM EFFECTS IN CHEMICAL REACTIONS OF POSITRONIUM

Yu.A. Berlin, I.B. Kevdina, and V.P. Shantarovich
Institute of Chemical Physics Academy of Sciences of the
USSR, 117334 Moscow, Vorobjevskoe Shausse 2b, USSR

Chemical reactions of positronium (Ps) in liquids proceed in three stages[1]:
Ps diffusion, formation of a Ps-reactant complex with subsequent stabilization
or decomposition in the wake of concommitant shrinking of the positronium "bubble".
Positronium diffusion is sometimes not considered as a separate step.[2]

Experiments are reported to investigate the role of quantummechanical Ps
tunneling between positronium "bubble" and potential well of the reactant in the
diffusion stage.[3] We measured ortho- to para-Ps conversion rates in $FeCl_2$ containing
water-glycerol solutions in the viscosity range 0.7 to 470 cp. The rates decline
with increasing viscosity toward a constant value for viscosities $\geq$ 70 cp. We
attribute this constant rate to viscosity independent positronium tunneling. By
contrast in the presence of a strong oxidizer ($K_2Cr_2O_7$) no such viscosity-indepen-
dent rates of positronium oxidation were observed.

The role of positronium tunneling in the temperature dependence of Ps chemical
reactions in liquids is explored.[4,5]

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POSITRON AGE-MOMENTUM CORRELATION IN SOME ORGANIC LIQUID

Y. Kishimoto and S. Tanigawa
Institute of Materials Science, University of Tsukuba,
Sakura-mura, Ibaraki 305, Japan

Correlation measurements between positron age and momentum of annihilation pairs were applied to benzene containing various concentrations of CCl_4 in order to clarify the formation mechanism of positroniums and the role of inhibitors in benzene. Figure 1 shows the block diagram of the measurement system. The time resolution was 540 psec (FWHM) when measured with a ^{60}Co source and the energy resolution was 1.7 keV for 512 keV line of ^{106}Ru. The channel width for time and energy were 53.6 psec and 480 eV, respectively. This system is ten times as fast as previous systems because of the use of the differential fast timing discriminators for start and stop pulses from photomultiplier tubes. In this work, the total triple coincidence rate was about 24 cps and it took 70 hours to accumulate 3×10^4 counts at the top of the two parameter map. Lifetime spectra were analyzed by two component fitting in each energy channel of Doppler broadening. The results in benzene are shown in Fig. 2. I_2 means the intensity of pick-off process of ortho positronium and τ_1 corresponds to the averaged lifetime other than pick-off process. This momentum dependence of τ_1 qualitatively resembles that in water, which will be presented in a separate paper at the conference. It is suggested that τ_1 consists of at least four components: $\tau_1(p)= \sum I^i(p)\tau^i$, where $\sum I^i(p) = 1$. When $\sigma^{(1)} < \sigma^{(2)} < \sigma^{(3)} < \sigma^{(4)}$ and $\tau^{(1)}, \tau^{(3)} < \tau^{(2)}, \tau^{(4)}$, the trends in τ_1 of Fig. 1 can be reproduced. These components may be assigned to the following processes: $(\tau^{(1)}, \sigma^{(1)})$ --- the self annihilation of completely thermalized para positroniums, $(\tau^{(2)}, \sigma^{(2)})$ --- the self annihilation of converted positroniums, $(\tau^{(3)}, \sigma^{(3)})$ --- the self annihilation of bound para positroniums and $(\tau^{(4)}, \sigma^{(4)})$ --- the other annihilation mode of positrons, where σ's are the parameters representing the width of momentum distibution. It was found that the two parameter correlation measurements are very powerful tool in understanding the formation and reactions of positroniums in organic liquids.
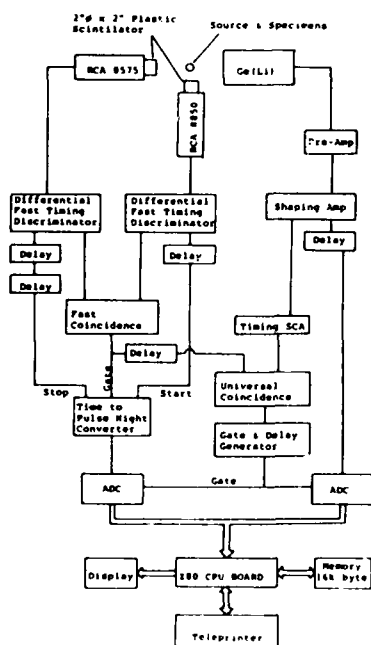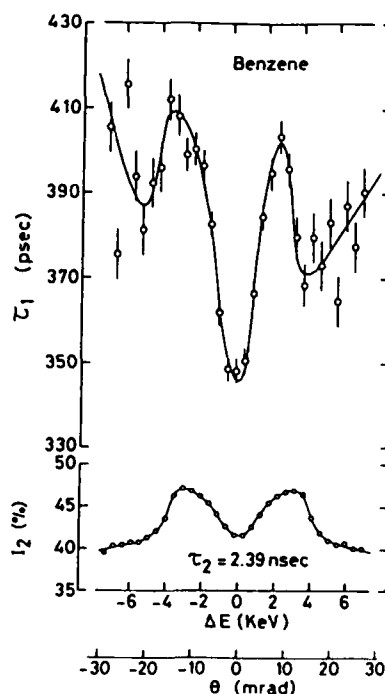

Fig. 1

Fig. 2

ANNIHILATION CHARACTERISTICS OF POSITRONS IN OXIDE POWDERS
IN THE RELATION TO CATALYTIC ACTIVITIES

K. Ito[#], Y. Ohtsu[#], S. Tanigawa[#] and N. Tsuda[##]

#)Institute of Materials Science, University of Tsukuba,
   Sakura-mura, Ibaraki 305, Japan
##)National Institute for Researches in Inorganic Materials,
   Sakura-mura, Ibaraki 305, Japan

The annihilation characteristics in some alkali earth metal oxide powders were studied by the measurements of Doppler broadening of annihilation radiations. MgO, CaO, SrO and BaO powders are well known as a solid base and are utilized as a catalyst for the reactions which start by extracting protons from molecules, such as the decomposition of alcohol. Figure 1 shows the lineshape parameter in MgO powders of the specific surface area of 35 m^2/g as a function of air pressure. Figure 2 shows the results of thermal equilibrium measurements of lineshape parameter under the vacuum of 10^{-6} torr. The heating and cooling runs are nearly the same. The baking at high temperatures in vacuum did not show any change in lineshape. Therefore, positrons in this case clearly observed the intrinsic surface of MgO. The temperature dependence in Fig. 2 can be considered as the thermal activation process of the escape of positrons from trapped surface states to form positroniums in accordace with the results by slow positron beam. Application of such surface escape model to data in Fig. 2 gave 0.187 eV for the activation energy of detrapping. Figure 3 shows the isochronal annealing behavior of the process $Mg(OH)_2 \rightarrow MgO$. This behavior is very similar to the cange in the number of basic points, specific surface area and catalytic activities in some reactions.
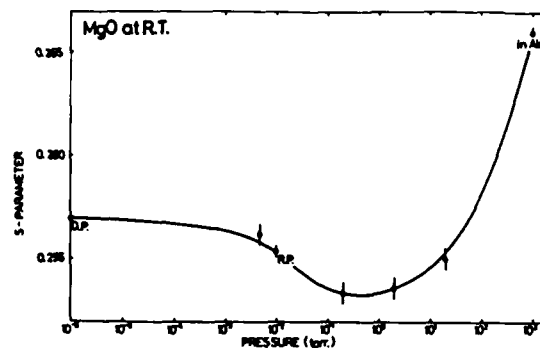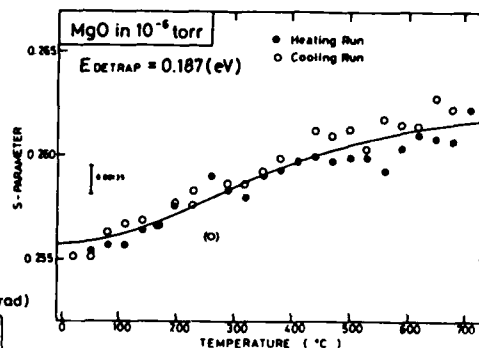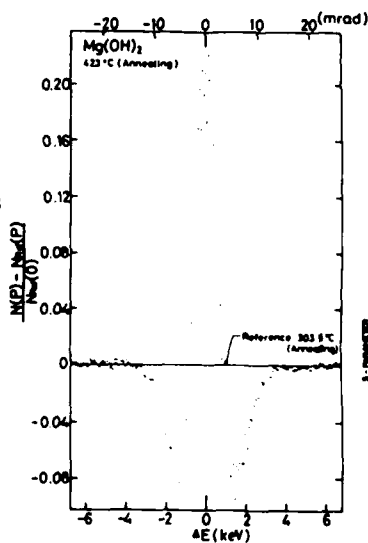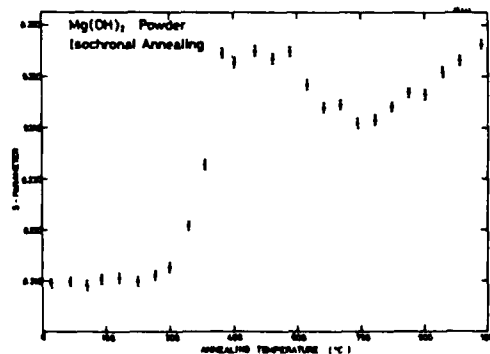

Fig. 1

Fig. 2

Fig. 4

Fig. 3

POSITRON AGE-MOMENTUM CORRELATION IN METAL OXIDE POWDERS
AS CATALYTIC MATERIALS

Y. Kishimoto,[#] K. Ito,[#] S. Tanigawa[#] and N. Tsuda[##]
#)Institute of Materials Science, University of Tsukuba,
    Sakura-mura, Ibaraki 305, Japan
##)National Institute for Researches in Inorganic Materials,
    Sakura-mura, Ibaraki 305, Japan

It has been suggested that the states of protons at the surface of catalytic materials may be simulated by positrons in a rough approximation.   In this paper, correlation measurements between positron age and momentum of annihilation pairs were carried out on MgO, SiO_2, ZnO and other oxide powders.   The momentum dependence of mean lifetimes (τ_M) in ZnO is shown in Fig. 1.   A maximum of τ_M at $\theta = 0$ suggests the existence of the annihilation mode which has the narrowest momentum distribution and the longer lifetime.   This mode seems to come from the ortho-para conversion process of ortho positronium.   After this process, converted para positroniums are completely thermalized.   In analyzing the lifetime spectra of ZnO, a long lifetime component ($\sim$1.2 nsec) appeared with a small intensity ($\sim$1%). This component is regarded as pick-off process of ortho positronium.   Since it is difficult to separate exaactly such component, it is included in τ_M.   On the other hand, the pick-off process was found to occur more frequently in MgO and SiO_2 powders as shown in Figs. 2 and 3.   In Figs. 2 and 3, τ_1 corresponds to a averaged lifetime other than pick-off process.   The change of τ_1 is common to MgO and SiO_2.   This momentum dependence can be explained by at least four annihilation modes, and is similar to the correlation spectra in water, ice and so on.   In the case of ZnO, the momentum dependence is similar to those in an aqueous solution of 3 mol/1 $MnSO_4$, ultrafine particles of nickel, gold and so on.   The close relation of the present results to catalytic reactions will be discussed.
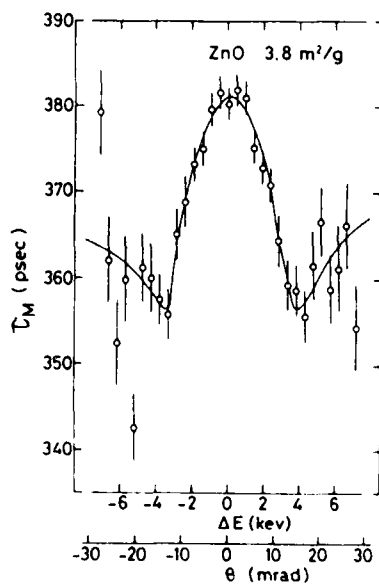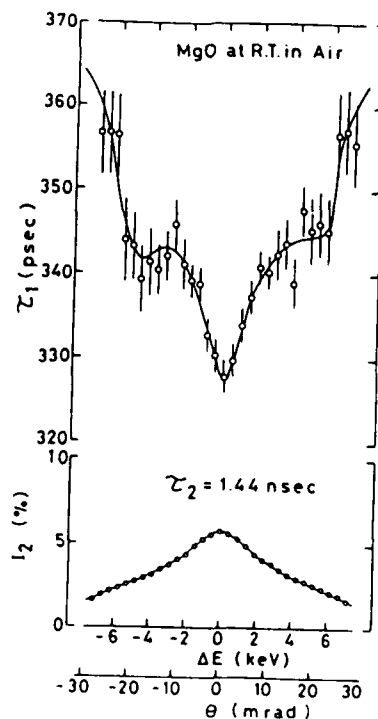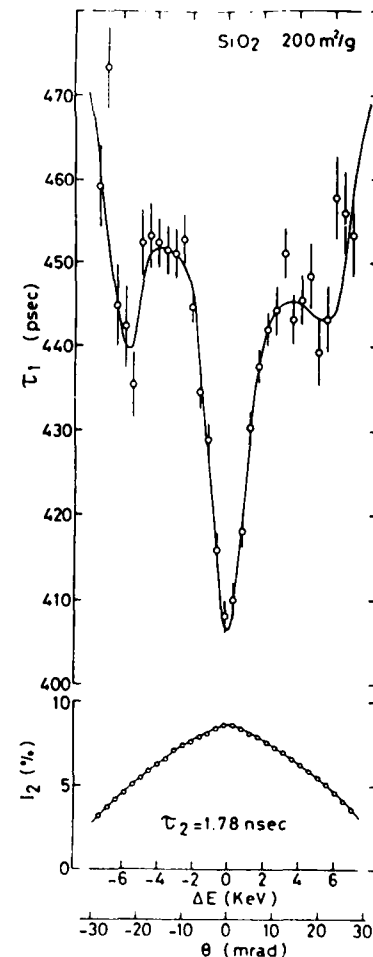

Fig. 1

Fig. 2

Fig. 3

DEPENDENCE OF PICKOFF ANNIHILATION

LIFETIMES ON DIELECTRIC CONSTANTS

M.G.Gaikwad[*], Sulabha Deuskar, S.K.David.
Department of Physics, University of Poona
PUNE - 411007, Maharashtra State, India.

A Direct relationship between ortho positronium
(o - Ps) pickoff annihilation lifetime and constitutive
physical property like dielectric constant for some
organic media has been reported. The validity of the
correlation has been checked for fifteen organic liquids.

[*] Permanent Address.
                K.T.H.M. College, Gangapur Road,
                Nasik - 422002, Maharashtra, India.

STUDY OF POLYELECTROLITE SYSTEMS
BY POSITRON ANNIHILATION TECHNIQUES

Sonia Millán S.
Subdirección de Investigación y Aplicaciones no Energéticas
Instituto Nacional de Investigaciones Nucleares
Benjamín Franklin 161, México 11, D. F., MEXICO

R. Zana
Centre de Recherches sur les Macromolécules
6, Rue Boussingault, 67084 Strasbourg-Cédex, FRANCIA

J. Ch. Abbé and G. Duplâtre
Centre de Recherches Nucléaires
23, Rue du Loess, 67037 Strasbourg-Cédex,   FRANCIA

The positron annihilation technique was applied to the study of polyion-counterion interactions in polyelectrolite systems. Cobalt dichloride was added to aqueous solutions of tetramethylammonium and sodium polysalts in order to investigate the interactions among the polyions and Co^{2+} ions (counterions) which are sensitively reflected in the positron annihilation parameters. Positronium lifetime changes abruptly at a certain Co^{2+} concentration in the solutions under study. This change is related with the amount of Co^{2+} ions which are capable of reacting with the polyelectrolite chain. The present results coincided with those previously reported by some other techniques. In a second series of experiments the positron annihilation technique was applied to investigate the interactions among polycations and periodate ions in aqueous solutions of polyvinyl-4-pyridine. The results concur with those predicted by Manning's Theory for polyelectrolite interactions |J. Chem. Phys., 51 (1969) 924|.

STUDY OF MICROEMULSION SYSTEMS
BY POSITRON ANNIHILATION TECHNIQUES. I

Rocío Reynoso V., Juan Serrano G., Belkacem Djermouni[a]
Luz Alicia Fucugauchi

Subdirección de Investigación y Aplicaciones no Energéticas
Instituto Nacional de Investigaciones Nucleares
Benjamín Franklin 161, México 11, D. F., MEXICO

In previous work we have reported on the application of positron annihilation techniques to the study of micellar aggregation phenomena in both aqueous and reversed micellar systems and the effect of increasing the amount of water solubilized in reversed micelles (leading to the formation of swollen micelles and eventually microemulsions) on the positronium formation probabilities.

In the present study positron annihilation techniques were applied to a more quantitative investigation of microemulsions consisting of sodium stearate-cosurfactant-water-oil (hydrocarbon) systems in which the solvent was isooctane or cyclohexane.

By varying subsequently the cosurfactant from n-butanol to n-pentanol and n-hexanol in all these systems an attempt was made to study the effect of the cosurfactant on the microemulsion formation process.

The effect of the surfactant concentration on the mechanism of microemulsion formation was also investigated. The results indicate that at higher surfactant concentration the ratio at which micro-emulsions are formed in isooctane-containing systems is larger than that ratio at which the same aggregates are formed at lower surfactant concentration in the same systems. The water solubilizing capacity of these microemulsions increases as a function of the surfactant concentration.

The positron annihilation data also sensitively reflect structural rearrangements in these solutions occurring upon further addition of water, such as the transition of spherical aggregates to a disk-like lamellae structures.

STUDY OF MICROEMULSION SYSTEMS
BY POSITRON ANNIHILATION TECHNIQUES. II

Rafael López C., Oscar Olea C., Luz Alicia Fucugauchi
Subdirección de Investigación y Aplicaciones no Energéticas
Instituto Nacional de Investigaciones Nucleares
Benjamín Franklin 161, México 11, D. F., MEXICO

The positron annihilation technique was applied to assess the effect of the double bond on the microemulsion formation mechanism by replacing the surfactant from sodium stearate to sodium oleate in surfactant-cosurfactant-water-oil (hydrocarbon) systems.

The effect of both oil and cosurfactant on the microemulsion aggregation process was investigated by substituting subsequently the solvent from isooctane to nonane and hexadecane and varying the cosurfactant (alcohol) chainlength.

Structures of these microemulsions have been assessed by considering the available conformation and shapes of the surfactant-cosurfactant-solvent assamblies.

Volumes of the same aggregates have been calculated by taking into consideration the packing constrain imposed upon kink formation.

The present results again demonstrate the sensitivity of the positron annihilation technique toward subtle rearrangements in liquid systems.

PERFLUORINATED NON-AROMATIC HYDROCARBONS. EFFECTIVE ELECTRON-SCAVENGERS WITH ANOMALOUS INFLUENCE ON THE YIELD OF o-Ps IN NON-POLAR SOLVENTS

Göran Wikander

Department of Physical Chemistry, University of Umeå, S-90187 Umeå, Sweden.

From steady-state scavenging experiments as well as electron impact investigations in the gas phase it has been found that many perfluorinated compounds are efficient electron scavengers, producing metastable molecular anions. From a spur-model point of view it is expected that electron scavenging with formation of molecular anions either should result in enhancement or minimum in the o-Ps yield. We have investigated $C-C_6F_{12}$, $C-C_7F_{14}$, C_6F_{14} and C_7F_{16} as concerns their influence on the yield of o-Ps in different non-polar solvents.[1-3] It appears that C_6F_{12} is a weak inhibitor in non-aromatic solvents, causing minimum in the o-Ps yield at $C \sim 0.1$ M. A further increase of the solute concentration enhances the o-Ps yield. However, when C_6H_6 is used as a solvent no minimum in the o-Ps yield is obtained. The minimum observed in the non-aromatic solvents is assumed to be due to the creation of molecular anions of C_6F_{12} upon scavenging of spur-electrons. In order to test this assumption further investigations were undertaken, where both C_6F_{12} and CCl_4 were used as additives in C_6H_{12}. The results reveal that a distinct "anti-inhibition" effect can be discerned when the "two-solute" system (CCl_4/C_6F_{12}) is compared with results from CCl_4/C_6H_{12} solutions. The effect is even more pronounced when the concentration of CCl_4 is fixed and the C_6F_{12}-concentration is varied.

Upon changing solvent to C_6H_6, it appears that no "anti-inhibition" effect is obtained. Instead we find that admixtures of the two solutes CCl_4 and C_6F_{12} increase the inhibition of o-Ps formation in C_6H_6 compared to results from CCl_4 dissolved in C_6H_6.

Preliminary results from investigations where the three other perfluorinated substrates have been used as additives reveal the following.

When used as additive in C_8H_{18}, it appears that the behaviour of $C-C_7F_{14}$ is very similar to that obtained for C_6F_{12}. However, the ability of C_7F_{14} to inhibit o-Ps formation is much higher compared to C_6F_{12}.

As concerns the two linear perfluorinated substrated we obtain the following a) For low solute concentrations, the additives behave as typical although rather weak inhibitors. The decrease in the o-Ps yield levels off at sufficiently high solute concentrations, approaching a first minimum at $C \sim 0.4$ M. b) a further increase of the solute concentration results in an enhancement of the o-Ps yield. This enhancement levels off and approaches a maximum at roughly $C \sim 2$ M. c)Dissolution of still greater amounts of the additives results in a second decrease in the o-Ps yield. This decrease levels off and approaches a second minimum at $C \sim 4$ M. The o-Ps yield is lower for this minimum compared to that obtained in the low concentration range. d) In the region where the perfluoro-substrate dominates, diluted to some extent by a non-polar solvent, we find a substantial increase in the o-Ps yield approaching I_2 for the pure perfluorinated substrate.

The second minimum resembles that obtained for high concentrations of C_6F_6 in C_6H_{14}. However, inhibition curves where two minima are obtained for the same inhibitor have not been presented before.

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WHY DO HALOGENATED HYDROCARBONS INFLUENCE THE PS YIELD
IN NON-POLAR LIQUIDS? THE INTERMEDIATE CASES!

Göran Wikander[*] and Ole Mogensen
Risø National Laboratory, Chemistry Department,
DK-4000 Roskilde, Denmark.
[*]Permanent address: University of Umeå, Department of Physical Chemistry,
S-90187 Umeå, Sweden.

For many years the mostly used strong Ps inhibitors in nonpolar liquids have been various chlorine, bromine, and iodine substituted hydrocarbons. More recently some of the fluorine substituted benzenes have been shown to enhance the Ps yield at the lower concentrations by the antirecombination effect in pure liquids, and by the antiinhibition effect if a strong Ps inhibitor is also added[1,2]. Partly triggered by the Ps yield results, radiation chemists have recently studied, in particular, hexafluorobenzene solutions in some detail[3,4]. It is reasonable to expect that some halogen substituted hydrocarbons influence the Ps yield in a way which is "intermediate" between the two extremes: Ps inhibition and Ps antiinhibition. The present paper presents results of a rather detailed investigation of some intermediate cases.

Radiation chemistry and Ps yield results indicate that the following processes occur in the positron spur in solutions of halogen substituted hydrocarbons, RX_n, $e^- + RX_n \rightarrow (RX_n)^- \rightarrow X^- + R\cdot$

$$e^+ + (RX_n)^- \rightarrow Ps + RX_n$$

$$e^+ + X^- \rightarrow [X^-, e^+]$$
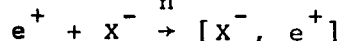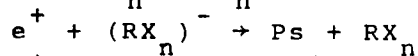
Hence, the trapped electron can form Ps only if $(RX)^-$ is stable or have a lifetime which is longer than or comparable to the Ps formation time of roughly 1 - 10 ps in nonpolar liquids. Apart from the flourine cases (X = F), where RX_n is stable, the lifetimes of RX_n^- against dehologenation are not known. Previous studies[5,6] have shown that some of the strongly chlorinated benzenes (n = 4 and 5) give reasonable Ps inhibition in benzene, but not in linear hydrocarbons. The reason is very probably that the dechlorination time is much larger in linear hydrocarbons than in benzene because Cl^- is more strongly solvated in benzene (a weak electron acceptor, higher polarizability) than in linear hydrocarbons. Maybe the RX_n^- anion complex with benzene plays a role, too.

Based on those results we have started detailed lifetime and angular correlation studies of solutions of the possible "intermediate", chlorinated benzenes.

By changing the solvent, e.g. from benzene to mixtures of benzene and hexane, or to mesitylene, xylene, etc., or by changing the substituents on the solute molecules we could show that the proposed interpretation seems to be in agreement with experimental facts. In the angular correlation work we try to find a $[Cl^-, e^+]$ component and its intensity in the angular correlation spectra. The estimated dehalogenation times might be measured by use of laser flash photolysis.

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COMPARISON OF ORTHO-Ps AND PARA-Ps FORMATION PROBABILITIES

O.E. Mogensen, F.M. Jacobsen, and M. Eldrup

Chemistry Department, Risø National Laboratory,
DK-4000 Roskilde, Denmark.

For liquids, in which Ps is formed, it is normally assumed that the ortho-Ps yield is equal to the relative intensity, I_3, of the longlived component in the positron lifetime spectrum apart from small corrections due to 3-γ decay. Similarly, the para-Ps yield is normally assumed to be equal to the relative intensity, I_N, of the narrow component in the angular correlation spectrum apart from small corrections due to pick off annihilation. The determination of the para-Ps yield from the lifetime spectrum is rather uncertain at present.

We have measured the positron lifetime and angular correlation spectra for 28 pure liquids in which Ps is formed, and for solutions of CCl_4 in hexane and diethylether and C_6F_6 in hexane. The angular correlation spectra could be well fitted by a sum of three gaussians with intensities (fwhm's) equal to: I_1 (2.4-3.0 mrad), I_2 (8.4-10 mrad), and I_3 (15-30 mrad), respectively. On assuming that $I_1 \simeq I_N$, the para-Ps contribution, we found the following results of comparing I_N with $I_3/3$ (both quantities corrected as mentioned above). 1) For 4 aromatic liquids $I_N \simeq I_3/3$ (e.g. I_N = 13.7%, I_3 = 43% for benzene). 2) For 10 linear and cyclic aliphatic hydrocarbons $I_N > I_3/3$ (e.g. I_N = 17%, I_3 = 42% for hexane). 3) For 3 ethers I_N is still larger than $I_3/3$ (e.g. I_N = 16.5%, I_3 = 30% for diethylether). 4) For 5 alcohols I_N is more uncertain, but $I_N > I_3/3$ (e.g. I_N = 8%, I_3 = 22% for ethanol). 5) For CS_2 I_N = 10.5%, I_3 = 44.5%. Other fits of the angular correlation curves will be discussed. The results for the solutions show how the ratio of I_N and $I_3/3$ depends on the Ps inhibition and "antirecombination" processes. Various models for a possible $I_N > I_3/3$ effect will be proposed, including the spur processes: 1) Ps^- formation, 2) oxidations of Ps by positive ions, and 3) ortho to para conversion on free radicals. The models can explain $I_N > I_3/3$ effects because of the longer ortho-Ps lifetime.

In summary our results seem to make plausible that the observed, apparent para-Ps to ortho Ps ratio is larger than three for many liquids. However, we cannot yet exclude that this effect is a result of the way we determine I_N.

COMPETITIVE HYDRATED POSITRON REACTIONS WITH HALIDES

O.E. Mogensen, J.R. Andersen, and N.J. Pedersen
Risø National Laboratory, Chemistry Department,
DK-4000 Roskilde, Denmark.

For some years the solvated positron (i.e. the "free" positron which does not form Ps) in liquids has been studied at Risø[1-3]. Mainly angular correlation measurements were used. This paper reviews recent results.

The rate constants of the hydrated positron reaction with I^- have been determined for $[I^-] \leq 0.03$ M in pure H_2O and in 1.74 M PPS (a Ps inhibitor) solutions of H_2O and D_2O. The rate constant was inversely proportional to the viscosity, as expected for a diffusion controlled reaction of a strongly hydrated reactant.

Hydrated positron reactions with halides in aqueous solutions of two halides were studied in detail. At halide concentration below roughly 0.03 M simple competition kinetics with previously determined diffusion controlled rate constants and with positron transfer from the more shallow to the deeper trap (i.e. the "two trap trapping model with transfer from shallow to deep trap") describe the results fairly well. The first positron transfer rate constants have been determined (e.g. 2×10^{10} M^{-1} s^{-1} for the $[Br^-,e^+] + I^- \rightarrow Br^- + [I^-,e^+]$ reaction). At high concentrations ($\gtrsim 1$ M) the thermalized positrons form "encounter pairs" with several halides in most cases, and hence the positron can always react with the halides having the strongest binding with the positron. For example, the addition of 1 M Br^- ions to a 1 M I^- aqueous solution does not change the angular correlation curve significantly (I^- is the deepest trap for positrons). The change from simple competition to "encounter pair" kinetics has been studied in some detail.

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TEMPERATURE EFFECTS ON THE POSITRONIUM FORMATION INHIBITION PROCESSES IN VARIOUS POLAR SOLVENTS

J. Talamoni, J.Ch. Abbé, G. Duplâtre, Ch.D. Jonah, A. Haessler
Université Louis Pasteur et Centre de Recherches Nucléaires
Laboratoire de Chimie Nucléaire
B.P.20, 67037 STRASBOURG Cedex (France)

In view of the still alive controversy between the hot atom model (1,2) and the spur model (3,4) of positronium formation, the search for temperature effects on the inhibition of Ps formation appears quite relevant. Generally speaking, no significant temperature effect is expected in terms of hot reactions, as the thermal energy input is negligible compared to the energy thresholds of the reactions supposedly involved in Ps formation and inhibition. On the contrary, temperature and viscosity changes must affect some of the processes occurring in the spur, such as localization and solvation, and any reaction betweeen entities associated to the fluid.

Five solutes and five solvents have been used. The former have been selected on the basis of their various behaviours towards Ps formation and/or of their nature : NO_3^- and $Te(OH)_6$, two "total" inhibitors, one charged and the other neutral, Tl^+ and Cl^-, two "limited" inhibitors probably acting by electron and by positron scavenging, respectively, and I^-, which usually shows combined inhibiting and enhancing properties. All solvents were polar and they were chosen due to known temperature effects on the electron solvation times and/or on the viscosity water, methanol, ethanol, ethyleneglycol and glycerol-water mixtures.

In most cases, there are significant temperature effects. The activation energies of the inhibition constants are compared to those for the viscosity and the overall results are discussed in terms of the various models of Ps formation.

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POSITRONIUM INTERACTIONS WITH PARAMAGNETIC SOLUTES

G. Duplâtre, A. Haessler, J.Ch. Abbé, J.C. Machado, A. Marques
Université Louis Pasteur et Centre de Recherches Nucléaires,
Laboratoire de Chimie Nucléaire
B.P.20, 67037 STRASBOURG Cedex (France)

It is rather surprising that Ps quenching reactions with paramagnetic solutes, especially the transition metal cations, have not been thoroughly investigated so far. Only a few results have been reported on the quenching rate constants : these were measured exclusively through the lifetime spectroscopy and the nature of the anion used is very often quite confusing (1).

We have undertaken a systematic study of the quenching reactions with Mn^{2+}, Co^{2+}, Ni^{2+} and Cu^{2+} in aqueous solutions, using both the lifetime spectroscopy and the Doppler broadening of the annihilation radiation line shape techniques. Also, we have reinvestigated the reactions of Ps with some paramagnetic radicals of the nitroxide type in water and in methanol, and in mixtures of these two solvents, previously studied by Goldanskii (2). The variations of the quenching reaction rate constants with temperature have been examined.

The data show that spin conversion reactions are almost exclusive with Mn^{2+}, while they are mingled with a significant percentage of complex formation reactions with the other cations. Knowing the mechanisms of the reactions involved, the inhibition constants for these ions have been derived. While the constant for Cu^{2+} is well in line with the value expected on the basis of the rate constant for solvated electron scavenging, this is not true for the other ions, which have comparatively lower inhibition constants.

The results for the 2,2,6,6 tetramethyl 4 hydroxy piperidine 1 oxyl radical are in fair agreement with Goldanskii's. The most striking feature is the change from spin conversion to oxidation reactions on passing from methanolic to aqueous solutions. Temperature effects on solutions of these free radicals show unexpected features.

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EVIDENCE FOR THE EXISTENCE OF WATER:
ETHANOL CLUSTERS FROM o-Ps YIELDS

F.A. Smith and C.D. Beling
Department of Physics, St. Bartholomew's Medical College,
Charterhouse Square, London EC1M 6BQ, U.K.

Studies of Ps formation and quenching in solutions are conveniently made as a function of temperature and solute concentration in attempts to gain insight into spur processes. When changes in the state of solute protonation are required however, the introduction of OH^- and H^+, together with their accompanying ions may mask the effects due to the solute alone, especially when the solvent is non-aqueous. It is of interest therefore to investigate the combined and separate effects of solvent, water and NaOH and arrive at quantitative correction factors which may permit the extraction of effects due to solute alone.

o-Ps yields and decay rates were measured in ethanol i) with pure water added up to a concentration of 16M and ii) with 1M and 2M solutions of NaOH added up to a maximum H_2O concentration of 24M. A three component lifetime analysis was carried out with a fixed free-positron lifetime of 0.39 ns.

The major factor in affecting the o-Ps decay rate was found to be the concentration of water, the results being largely independent of the presence of NaOH. In all the solutions studied the decay rate could be ascribed to pick-off quenching, the data showing adequate agreement with the relations proposed by Tao[1] and Lévay and Vértes[2]. There is evidence however, of deviations at certain concentrations. The o-Ps yield showed a general enhancement as H_2O concentration was increased, with the maxima of small superimposed oscillations occurring at the same concentrations (Fig. 1) at which deviations were observed in the decay rate.

Although the electron moderation time is longer in ethanol, with a correspondingly longer spur length than in water,[3] the electron mobility is higher in water[4] and may be the dominant reason for its larger yield. If this is so, the yield minima at water concentrations of 3M, 8M and 18M could be due to states of minimum electron mobility and greatest liquid disorder. A (1:4)(H_2O:EtOH) molecular cluster would be expected to occur between 3M and 8M, and a (1:1)(H_2O:EtOH) cluster between 8M and 18M, producing greater order in the liquid structure and consequently a higher electron mobility.

Similar effects have been observed in the water:dioxane system by Brauer et. al.[5].
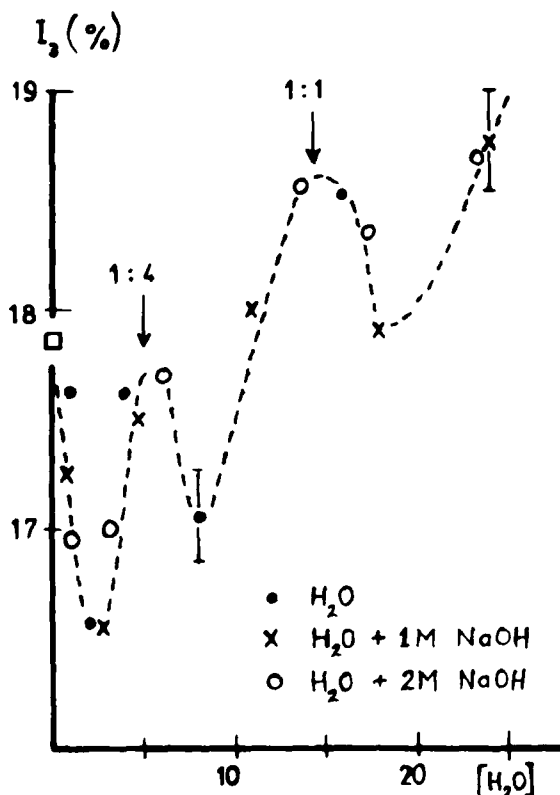
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CORRELATION OF DIELECTRIC RELAXATION AND
POSITRON ANNIHILATION IN SOME GLASS FORMING LIQUIDS

Bansi D. Malhotra and Richard A. Pethrick
Department of Pure and Applied Chemistry
University of Strathclyde, Thomas Graham Building,
Cathedral Street, Glasgow G1 1XL, Scotland

In a recent paper[1] on the positron annihilation a sigmoidal shaped curve was observed for the variation of the ortho-positronium lifetime with temperature for orthoterphenyl. A similar shaped curve had previously been observed for the glass-forming phenyl ether liquids[2]. The lower temperature elbow is associated with the glass transition temperature (T_g) for these systems and is associated with the generation of free-volume in the system. The higher temperature elbow has been the source of some recent speculation. It is however shown in this paper that the temperature at which this transition occurs coincides with that at which the dielectric relaxation of these systems has a characteristic frequency which is of the same order of magnitude as the time constant for the ortho-positronium lifetime[3]. This observation supports the hypothesis that the change in the temperature dependence of the curve is associated with dynamic changes in the volume containing the ortho-positronium. A theoretical analysis of this situation is currently being developed and will be presented.

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MAGNETIC FIELD QUENCHING OF POSITRONIUM IN ORGANIC LIQUIDS

Sunant Rochanakij and D. M. Schrader
Chemistry Department
Marquette University
Milwaukee, WI 53233, U.S.A.

The objective of this research is to understand better the formation and decay of positronium in organic liquids. A fast-fast coincidence system is used for measuring positron lifetime spectra. Specifically, the dependence of intensity and decay rate of positronium in neopentane and tetramethylsilane (TMS) as a function of external magnetic field will be reported for different concentrations of quenching solutes. Exploratory observations on the effect of a superimposed electromagnetic field in the microwave region are being investigated.

PHOTOMAGNETIC QUENCHING OF POSITRONIUM IN ORGANIC SOLUTIONS

David A. Diehl and D. M. Schrader
Chemistry Department
Marquette University
Milwaukee, WI 53233, U.S.A

Photomagnetic quenching of positronium by phosphorescent molecules through spin conversion of the excited triplet state has been reported by Brandt and coworkers in solids and gases. Extremely large cross-sections for this phenomenon are observed. We are examining this effect in organic liquids containing phosphorescent solutes to obtain the interaction cross-sections and their relationship to the properties of the medium, and the chemical structure of the phosphor. Of interest is the nature of the excited phosphor, including the triplet state energy and lifetime, singlet state lifetime, and type of transition. Results for acetone solutions in cyclohexane will be presented.

COMPARISONS OF POSITRONIUM AND MUONIUM ATOMS
IN CONDENSED MATTER

Y. C. Jean*
Department of Physics, University of Missouri-
Kansas City, Kansas City, Mo. 64110
Y. Ito
Research Center for Nuclear Science and Technology
University of Tokyo, Tokyo, Japan
J. M. Stadlbauer, B. W. Ng and D. C. Walker
Department of Chemistry and TRIUMF, University of
British Columbia, Vancouver, B.C., V6T 1Y6, Canada

Positronium (Ps) and Muonium (Mu) atoms are considered to be the
superlight and the very light isotopes of hydrogen atoms. We compare
these two light atoms in terms of chemical kinetics, formation mechanisms
and practical applications as nuclear probes in liquid phases. Ps atoms
show similar chemical reaction kinetics as Mu and H atoms for diffusion-
controlled reactions but different reaction kinetics for thermally acti-
vated reactions. The formation mechanisms for Ps and Mu seem quite
different. Mu is believed to be mainly formed by "hot" processes while
Ps is often reported to be formed after thermalization. The practical
applications of these two atoms for the investigation of structural
chemistry are discussed. One probe complements the other.

THE SOLVATED POSITRON; TOWARDS A THEORY

Paul E. Cade and Chih-Mai Kao
Department of Chemistry, University of Massachusetts
Amherst, Massachusetts 01003, U.S.A.

The hydrated positron is considered an established entity in positronium chemistry. Lifetimes, angular correlation curves, $N(\Theta)$, and Doppler broadening spectra have been presented for the hydrated positron and are routinely attributed to this species. The dynamics of the positron behavior in condensed media has been explored by discussion of various solvation stages, from 'dry' to 'wet', in close parallel with related picosecond experiments involving the solvated electron. Much of the work to date involves water as the solvent, but a general phenomena is implied. In case of the hydrated, or solvated, positron, optical spectra is unavailable to follow solvation stages and EPR of positrons trapped in glasses is not feasible in order to consider the 'structure' of these systems – these methods have provided much vital information on the solvated electron. It is tempting to consider much of the knowledge of nature of the solvated, or trapped, electron to be generally applicable to the case of the positron and this perspective dominates consideration of the solvated positron (The solvated proton plays a minor role). It is desirable, however, to consider the nature of the solvated positron in terms of a local solvent structure (if applicable), solvation energies, mobility, and annihilation behavior in a direct sense. This paper contributes to a beginning with ab initio quantum mechanical calculations on various model systems. Other general, or delocalized, perspectives are also possible.

In contrast to the case of the solvated electron, it is necessary to obtain a wavefunction for the electrons surrounding the solvated positron in order to perform calculations on annihilation properties. We present a three stage approach to a general consideration of the solvated positron;

i.) Calculations involving a model potential for the positron, e.g. a semi-continuum theory, are elementary and yield a positron wavefunction given certain assumptions about the trapping potential. This positron function can then be used together with a free solvent molecule wavefunction – assuming additivity of contribution to annihilation and a solvation structure – to obtain annihilation properties. This approach is formulated and its' merits and difficulties are summarized.

ii.) At a second level, the solvent is given explicitly for the first solvation shell, e.g. the complex system, $(H_2O)_n e^+$, is considered as a 'cluster' system. This requires a model of the solvation situation with the number, location, and orientation of the solvent molecules assumed or explored. At this level, inclusion of more solvent molecules, in addition to the n molecules in the 'cluster', can be attempted in an approximate fashion as described. Newton,[1] Morokuma and Noell,[2] and Kestner[3] have considered such calculations for the solvated electron and our studies parallel their studies in many (but not all) respects. We will summarize the annihilation properties as a function of the solvation structure and other parameters of the system.

iii.) A third stage attempts to couple a phenomenological theory with an ab initio calculation. This basic approach is to consider the first (and perhaps second) solvent shell and the positron in an explicit ab initio approximate Hartree-Fock study and then with suitable potentials relax the solvent within the neighborhood of the 'cluster-berg', $(H_2O)_n e^+$ much in the same fashion that ion hydration is currently studied by Monte Carlo simulation with assumed potentials. This general approach is outlined and results summarized as available.

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Paul E. Cade and Chih-Mai Kao
Department of Chemistry, University of Massachusetts
Amherst, Massachusetts 01003, U.S.A.

Mogensen and Shantarovich[1] have presented evidence for the existence of [X⁻:e⁺] systems in aqueous solutions and subsequent research has extended this study and also examined competitive reactions.[2,3] These authors present angular correlation curves, $N(\theta)$, for these positron/halide-ion systems, except for [F⁻:e⁺], and find the order of relative stability reversed from that predicted theoretically for the free gaseous systems.[4] It appears that these systems are among the better characterized positron/molecule complexes in positronium chemistry.

In theoretical calculations Cade and Farazdel[4] give angular correlation curves, $N(\theta)$, which agree very well with the experimental results for the [Cl⁻:e⁺], [Br⁻:e⁺], and [I⁻:e⁺] systems. However, the theoretical results are for gas phase (vacuum) entities and one expects that solvent effects will influence the behavior of these tenuous systems. The present paper probes the influence of solvent molecules in the proximity of the positron/halide-ion system on the positron affinity and the annihilation properties; the focus is on the [F⁻:e⁺] and [Cl⁻:e⁺] systems. We present ab initio approximate Hartree-Fock calculations on cluster systems such as $[(H_2O)_n X^-:e^+]$ where X⁻ is F⁻ and Cl⁻ and n takes values from 1 to 4 or 6. In these calculations we take the best available data for the solvation structure of the F⁻ and Cl⁻ ions in water and then attach a positron to this system. This is done in stages to gauge the progressive effects of adding water molecules, e.g. by study of $[H_2O-F^-;e^+]$, $[(H_2O)_2F^-;e^+]$, $[(H_2O)_3F^-;e^+]$, and $[(H_2O)_4F^-;e^+]$ sequence. The experimental evidence suggests a solvation shell of four water molecules for F⁻ and six water molecules for Cl⁻ and this is taken into consideration. The electronic basis sets used in these calculations are large, but not exhaustive, but the positron basis set is probably adequate within the approximations employed.

The calculations indicate a considerable decrease in the positron affinity to the X⁻ ion when water molecules are present and it appears this effect is cumulative to solvent shell completion. The positron affinity decreases by values of up to 30-40% when the total energy of the cluster is minimized - i.e. the positron affinity is apparently not a major factor in stabilizing the cluster and it can be increased (from the free system value) only by unacceptable increases in the energy of the (small) cluster. Obviously a more complete solvent relaxation is needed to understand this behavior. The two-gamma angular correlation curves, $N(\theta)$, have been computed, at present, for the [X⁻:e⁺] systems in the presence of only one and two neighboring water molecules. We find that the angular correlation for the $[H_2O-F^-;e^+]$ and $[(H_2O)_2-F^-;e^+]$ systems are perceptibly narrower than for the free gas system [F⁻:e⁺] and a parallel behavior is noted for the [Cl⁻:e⁺] system. It is our impression that shift to a narrower $N(\theta)$ is cumulative and our calculated $N(\theta)$ for the fully solvated species would be significantly different from the measured angular correlations. In these calculations, we have not at this time attempted to 'relax' the cluster, i.e. to permit expansion about the neutralized system and allow solvent molecule re-orientation. It remains possible that when these variables are taken into account the [X⁻:e⁺] systems may occupy a 'bubble' of volume such that the influence of neighboring solvent molecules are now greatly reduced. This possibility is now being explored.

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A PHASE TRANSFORMATION STUDY OF
n-HEXADECANOL BY POSITRON ANNIHILATION

William W. Walker
Department of Physics and Astronomy
The University of Alabama, University, Alabama 35486, U.S.A.

Positron lifetimes have been measured as a function of temperature in n-hexadecanol (cetyl alcohol). This fatty alcohol is known from x-ray diffraction experiments to have at least three crystal forms, and the presence of these crystal forms has been observed by various other techniques.[1] The present measurements examine the sensitivity of positron lifetimes to changes in the crystal structure of n-hexadecanol.

The three solid forms of n-hexadecanol are: α (hexagonal), β (orthorhombic), and γ (monoclinic). Both the β and γ forms are stable at temperatures well below the melting point while α is a waxy phase stable for only a few degrees below the melting point. The $\beta \rightarrow \alpha$ transition occurs at 42°C, the $\gamma \rightarrow \alpha$ transition occurs at 46°C, and the α phase melts at 48.6°C.

Samples of n-hexadecanol which have been crystallized from various solvents or from the melt at different cooling rates have been examined by x-ray diffraction, differential scanning calorimetry, and positron lifetime measurements. The fact that the β and γ phases commonly co-exist complicates the analysis of experimental results. It is found that positron lifetime parameters differ only slightly for the β and γ phases as might be expected since their unit cell dimensions are quite similar. Although β and γ phases show only a slight temperature dependence, the hexagonal α phase exhibits a strong temperature dependence.

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SURFACTANT VESICLES STUDIED
BY POSITRON ANNIHILATION TECHNIQUES

Juan Serrano G., Rocío Reynoso V., Luz Alicia Fucugauchi
Subdirección de Investigación y Aplicaciones no Energéticas
Instituto Nacional de Investigaciones Nucleares
Benjamín Franklin 161, México 11, D. F., MEXICO

The positron annihilation technique was applied to assess the occurrence of thermotropic phase transitions in aqueous solutions of surfactant vesicles formed by ultrasonic dispersion of $[CH_3(CH_2)_{15}]CH_2=CH(CH_2)_8CONH(CH_2)_6\overset{+}{N}(CH_3)_2$, Br^- and its analogs polymerized either by azoisobutyronitrile (AIBN) or by ultraviolet irradiation.

Positron lifetime measurements were performed in all three solutions as a function of temperature. The results indicate that both polymerized vesicles and their unpolymerized counterparts undergo several phase transitions at different temperatures.

The annihilation parameters measured in these systems also reflect that the temperatures at which the vesicle polymerized by AIBN undergoes phase transitions differ from those at which the transitions occur in the UV polymerized vesicle which might be associated with the different polymerization rate belonging to each one of them.

STUDIES OF PHASE TRANSITIONS IN
POLYETHYLENE TEREPHTHALATE POLYMERS BY
POSITRON LIFETIME TECHNIQUE

P. K. Tseng, S. P. Chang and S. Y. Chuang*
Physics Department, National Taiwan University
Taipei, Taiwan, China

Lifetime spectra of positron annihilation in polyethylene terephthalate (PET) have been measured as a function of temperature from -196°C to 100°C. All lifetime spectra were decomposed into two lifetime components. The lifetime τ_2 and the intensity I_2 of the long lifetime component increased with increasing temperature T. It was found that the slope of the τ_2 vs. T curve changes at the following temperatures: 60°C, -80°C, and -160°C. The value of I_2 also showed a marked change at 60°C and -80°C but remained constant from -80°C to -196°C. Those changes detected by positron lifetime measurements are attributed to microscopic changes due to rotations of various chains in the polymer.

*Present address: Department of Physics, University of Texas at Arlington, Arlington, Texas 76019, U.S.A.

DETECTIONS OF PHASE TRANSITIONS IN
NaNO$_3$ CRYSTALS BY POSITRON ANNIHILATION

S. Y. Chuang, M. E. Ottlinger, L. M. Diana
P. G. Coleman, S. C. Sharma and J. Smith
Center for Positron Studies, Box 19059, UTA Station
The University of Texas at Arlington, Arlington, TX 76019, U.S.A.

Lifetime spectra of positron annihilation in polycrystalline NaNO$_3$ powders have been measured as a function of temperature from 200°K to 560°K. All lifetime spectra were decomposed into two lifetime components, a short lifetime component with meanlife τ_1 ranged from 250 psec to 280 psec and a long lifetime component with meanlife $\tau_2 \sim 1.2$ nsec and a small intensity $I_2 \sim 1.2$ nsec and a small intensity $I_2 \sim 0.5\%$. It was found that ζ_1 undergoes a drastic change at about 540°K which may be attributed to the onset of disordered vibration-rotation of the nitrate group in NaNO$_3$.[1] It was also observed that a small change in ζ_1 occurred at about 250°K $\sim$ 270°K which seems to confirm the new phase transition observed by x-ray studies.[2] Samples of NaNO$_3$ single crystals are currently under investigation and the result will also be presented.

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HIGH-SPIN - LOW-SPIN TRANSFORMATION OF 3 d TRANSITION METAL IONS INVESTIGATED BY POSITRON ANNIHILATION

A. Vértes[+], Zs. Kajcsos[++], L. Marczis[++]

[+] Department of Physical Chemistry and Radiology, Eötvös Loránd University, H-1088 Budapest, Hungary
[++] Central Research Institute for Physics, H-1525 Budapest, P.O.B. 49, Hungary

The positron lifetime spectra were recorded in aqueous solution of 3 d transition metal ions in high-spin and low-spin state. The increase in the concentration of the high-spin metal ions resulted in a decrease of the average lifetime of the ortho-positronium, while low-spin ions were inert for the ortho-positronium lifetime. This results proves that the character of the interaction between the studied paramagnetic ions and the ortho-positronium is an ortho-para conversion.

OBSERVATION OF PHASE TRANSITIONS IN BUTADIENE-STIRENE COPOLYMER BY POSITRON LIFETIME MEASUREMENT TECHNIQUE

P.U.Arifov,S.N.Vasserman,A.A.Dontsov,S.A.Tishin
Arifov Institute of Electronics,Academy of Sciences Uz.SSR
700052,Tashkent,Observatorskaja,85,USSR

It is known that the butadiene-stirene block-copolymer (DST) has the two-phase segregational structure.Unlike DST the butadiene stirene rubber (BSR) has the monophase structure with the statis - tic distribution of butadiene and stirene links in the macromole - cular chain.
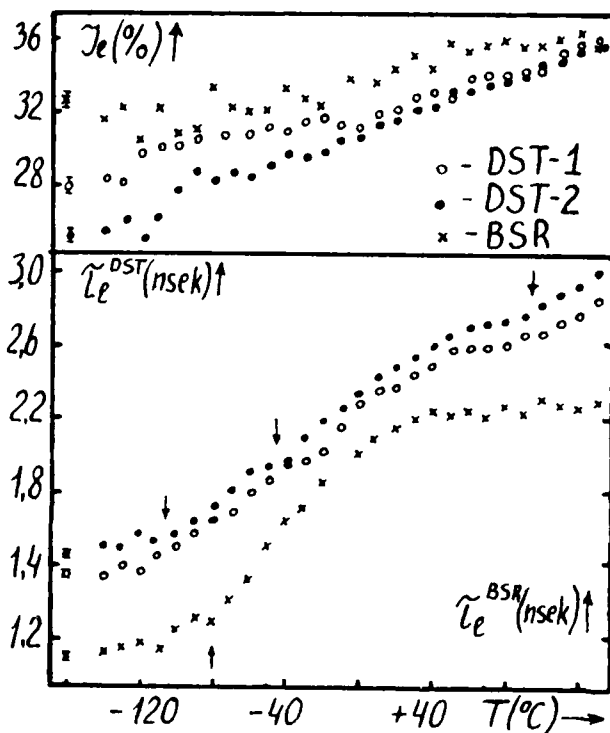
The results of the measure- ments of the temperature depen - dence of lifetime τ_ℓ and the in- tensity of long-lived component J_ℓ of the lifetime positron spect - rum in BSR (stirene content is 25%), DST-I and DST-2 (stirene content is 30% and 50%, respec - tively) are shown in Figure.The positron lifetime was measured with the fast-slow spectrometer (FWHM = 4IO p sec.).The samples were annealed at T =+IIO°C (du- ring 8 hours) before the measu- ments.The cooling rate of the samples in the measurements was not more than 2.5°C per hour.

The structure transitions connected with the glassing pro- cesses are clearly seen on the temperature dependences τ_ℓ . If BSR has the only glass-transiti- on connected with the rubber glassing (-80°C) the curves of DST have two folds one of which corresponds to the polybutadiene blocks and the other (+ 90°C) to polystirene blocks.

In addition the third temperature transition is seen on the temperature dependences τ_ℓ for DST at-50°C which is probably connec- ted with the intermidiate phase glassing. This phase is formed due to the mutual penetration of macromolecular segments on the bounda- ry of phase separation of rubber matrix and the polystirene blocks. The observed transition in DST-2 is more obvious because of the volu- metric fraction of the transition layer.

Noticeable decrease of J_ℓ in DST at the temperature lowering also indicates the existence of the transition layer with the in - creased packing density. According to our data the numeric estima- tions showed that the volumetric fraction of these regions was 7% for DST-I and I8% for DST-2. It should be noted that the interpre- tation of the found effect of the change of τ_ℓ temperature depen - dence slope near 0°C for BSR can be given under the comparison with Boyer data /I/ and the observed fold is probably connected with the structure transition in highly elastic state.

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SEARCH FOR THE CHARGE DENSITY WAVE IN SOLIDS BY POSITRONS: A TASE2 CRYSTAL

Y. C. Jean*

Department of Physics, University of Missouri-
Kansas City, Kansas City, MO.

An attempt to detect the Charge-Density-Wave (CDW) phase transitions has been made in an annealed $2H-TaSe_2$ crystal by the positron lifetime method. The positron lifetimes of this crystal were carefully measured as a function of temperature between 10 and 598 K. Two distinct and constant lifetimes, i.e. $0.130 + 0.007$ nsec and $0.378 + 0.008$ nsec, were found in the temperature range between 10 K and 300 K. These two lifetimes are thought due to the anisotropy character of the two-dimensional layered structure of the crystal. Positrons appear too localized to detect and CDW modulations in this crystal.

POSITRON ANNIHILATION IN A HOMOLOGOUS SERIES OF LIQUID CRYSTALS

J.K. Nash, J.D. McNutt, S.C. Sharma, L.M. Diana, S.R.S. Kafle, P.G. Coleman
Center for Positron Studies, Box 19059, UTA Station
The University of Texas at Arlington, Arlington, Texas 76019, USA

Positron lifetime spectra have been measured for several members
of 4,4'-di-n-alkoxyazoxybenzenes, a homologous series of nematic
liquid crystals. The lifetime spectra were measured as a function
of temperature from solid to isotropic liquid phase, and resolved into
a maximum of four lifetime components.
The observed behavior of the resolved annihilation parameters
can be interpreted in terms of changes in the intermolecular forces.

DETECTORS FOR POSITRON LIFETIMES MEASUREMENTS
- A NEW CONCEPTION

A.J.Salamon
Institute of Physics and Chemistry of Metals
Silesian University 40-007 Katowice, Bankowa 12, Poland

Abstract:

A new scintillation system - a thin plastic scintillator with heavy metal foil posited on its surface has been designed and tested.

It is well known that scintillators shows an improvement in time resolution, when the crystal height is reduced. But yet a counting efficiency is then lowered.

An improvement in counting efficiency has been found for the thin plastic scintillator with optimum thickness Pb foil placed on the scintillator surface. In high energy region of the energy spectrum has been observed greater counts rates comparatively to energy spectrum of the thin or large scintillators. A comparative study of the thin plastic scintillators with Pb foil /24mm ø x 6mm plus 0.5mm Pb foil for start detector and 24mm ø x 2mm plus 0.1mm Pb foil for stop detector/, conical /24mm base diameter, 8mm top diameter and 25mm height/ and cylindrical scintillators /24mm ø x 25mm/ has been performed.

A comparison of the timing and counting performances of this three types of the scintillator shapes shows, that the time resolution and counting efficiency /for energy window 20%, of the ^{60}Co Compton spectrum/ of the thin scintillators with Pb foil are as good as for conical and are better then for cylindrical scintillators. The improvement factor of the counting efficiency for the thin scintillator with Pb foil comparatively to the thin scintillator without Pb foil have values: about 15 for stop detector /for energy window 20% of the ^{137}Cs Compton spectrum/ and about 2 for start detector /for energy window 20% of the ^{60}Co Compton spectrum/.

IN SITU SOURCE GENERATION FOR
POSITRON LIFETIME MEASUREMENTS

J.D. McGervey and B.S. Chandrasekhar

Department of Physics, Case Western Reserve University, Cleveland, Ohio 44106

J.W. Blue

NASA Lewis Research Center, Cleveland, Ohio 44115

Application of the _in situ_ technique to positron lifetime measurements eliminates the often difficult problem of source component analysis. Previous work using this technique has been restricted to samples containing $A\ell$ and Mg.[1] Consideration of other nuclear reactions shows that there are other possibilities. Irradiation of Si with high energy protons results in the production of ^{22}Na via the reactions $^{29}Si(p,2\alpha)^{22}Na$ and $^{28}Si + p \rightarrow {}^{4}He + {}^{3}He + {}^{22}Na$; irradiation of Ni produces the positron emitter ^{58}Co via the reaction $^{61}Ni(p,\alpha)^{58}Co$. We have used this technique to produce $30\mu Ci$ of ^{22}Na in a 0.17g sample of V_3Si; the lifetime spectrum of the resulting positrons was devoid of any detectable source component. We now plan to irradiate a sample of nickel, and to use the resulting ^{58}Co to measure positron lifetimes in annealed Ni and in Ni containing defects. Further possibilities might become apparent if one looked for other reactions resulting in the production of ^{4}He and ^{3}He.

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COMPUTER INFORMATION SYSTEM ON POSITRON ANNIHILATION

Arifov P.U., Malyan V.M., Tolpegina L.S., Umarova F.T.

Arifov Institute for Electronics, Tashkent, USSR

In 1975 a bibliography for literature for the period 1930-1974 on most aspects of the chemistry and physics of low energy and thermalized positrons and positronium was published by R.M.Lambrecht / I /. The compilation contained 2449 entries for contributions of I779 authors. Lambrecht showed the phenomenal growth of the study of positron annihilation and predicted the growth rate during the next years. Now we observe this predicted picture. Therefore it is very important to compile and summarise information on positron and positronium.

In I968 first experimental data tables were listed / 2 /. Later, Positron-Annihilation Data, Tables I, II and III for experimental data measured by techniqes of two-photon angular correlation, positron annihilation life-times and Doppler broadening of annihilation-radiation line shape were published in Atomic Data and Nuclear Data Tables / 3,4 /.

Computer Information System for collection, keeping and search information on positron and positronium annihilation has been developed and tested in Institute for Electronics in Tashkent. Each document of system has bibliography description, abstract and search parts for automatic selection information.

The information sources include VINITI PEFERATIVNYI ZHURNAL "FIZIKA", "KHIMIYA" (I954-I980), abstracts of the papers presented at the Third and Forth International Conference on Positron Annihilation. The compilation contains about 5 000 documents. There is the bibliography published by Lambrecht in system separately.

In addition to our computer based data system we suppose to include Positron-Annihilation Data / 3,4 /, abstracts of the International Nuclear Information System (INIS), Chemical Abstracts and short versions of proceedings of the next International Positron Annihilation Conference.

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A Method of Estimating the Positron
Annihilation Line Shape

Cao Bi-song[a], Wang Yun-yu[b]

a) Tsinghua University, Department of Engineering and
   Physics, Peking, China
b) Institute of High Energy Physics, Acadimia Sinica,
   Peking, China

A method of estimating the positron annihilation Line Shape S and
H Parameters in perfect pure metals under the concrete experimental
condition is presented. In order to examine the reliability of this
method, we have measured the Line Shape parameters S and H of 15 kinds
of annealed metals. The estimated values of all the metals except Cd
are in good agreement with the results of experimental measurements.
The deviation of Cd has been discussed.

The energy distribution of the annihilation photos can be described
as following expression

$$I_0(E) = \frac{3k}{4fr_m}\sqrt{\frac{mc^2\pi}{E_F}}\,h_G\left(1-\frac{2E^2}{mc^2E_F}\right) + h_G\,e^{-\frac{2r_m^2}{m^2c^4\hbar^2}E^2} \qquad \left(|E| \le \sqrt{\tfrac{1}{2}mc^2E_F}\right)$$

$$I_0(E) = h_G\,e^{-\frac{2r_m^2}{m^2c^4\hbar^2}E^2} \qquad\qquad \left(|E| > \sqrt{\tfrac{1}{2}mc^2E_F}\right)$$

The resolution function of the Ge(Li) detector is considered and convo-
luted with them. Then we get the mathematic expression of the annihila-
tion peak distribution I(E)

$$I(E) = \int_{E+\frac{1}{K}}^{E-\frac{1}{K}} g\,h_G\left(\frac{K^2}{2a^2}+K^2E^2-1\right)e^{-a^2x^2}dx \;+\; \frac{g\,h_G K^2}{2a^2}\left(E+\frac{1}{K}\right)e^{-a^2(E-\frac{1}{K})^2}$$

$$+\; \frac{g\,h_G K^3}{2a^2}\left(\frac{1}{K}-E\right)e^{-a^2(E+\frac{1}{K})^2} \;+\; \frac{h_G}{\sqrt{2}\,b\sigma}\,e^{-\frac{E^2}{2\sigma^2}}$$

where coefficients a,b,σ,k,g are interrelated with the Fermi energy E_F
the ionic radii r_m of the metals, the ratio f of the positron annihila-
tion on the core and free electrons, and the resolution of detector
(FWHM).

The present work provided a method of estimating ratio f of the
positron annihilation on the core and free electrons according to
measuring the S and H parameter, need not unfolding the annihilation
spectrum.

The Measurement of Positron 3γ Annihilation
with the Ge(Li) Detector

Wu Gun-hong, Tang Xiao-wei, Wang Yun-yu

Institute of High Energy Physics, Acadimia Sinica
Peking,China

A method of determining the yield ratio of 3γ and 2γ annihilation P_3/P_2 is presented, on the basis of measuring the 5II kev annihilation peak counts of the investigated sample and the reference sample (annealed Al) with Ge(Li) detector. This method is called the "peak method".

$$\frac{P_3}{P_2} = \frac{3\gamma \text{ yield of the investigated sample}}{2\gamma \text{ yield of the investigated sample}} = \frac{\overline{Ip} - Ip - Ip/372}{Ip}$$

$$= \frac{\overline{Ip}}{Ip} - \frac{37I}{372}$$

where $\overline{Ip}$ and Ip represent the total counts of the 5II kev gamma peak of reference and investigated sample, respectively.

Another method called the "peak-valley method" has also been investigated, where not only the 5II kev peak, but also the valley part of the annihilation gamma specta are carefully measured.

$$\frac{P_3}{P_2} = \frac{Iv - KI_\rho}{\eta \xi \, Ip} \quad , \qquad K = \frac{\overline{Iv}}{Ip}$$

where $\overline{Iv}$, Iv represent the counts in a special valley region of the reference and investigated sample, respectively, η is the ratio of averge detection effeciency, ξ represent the 3γ fraction of that special valley region in the whole spectrum.

The peak method is more accurate and simple than the peak-valley method.

Using these two methods, the yield ratios of 3γ and 2γ annihilation in the MgO, teflon and α- $LiIO_3$ single crystal samples were measured experimentally. The value of the yield ratio in the α- $LiIO_3$ is $(I.05 + 0.20) \times 10^{-2}$.

A MICROPROCESSOR-BASED ACAR SYSTEM

C. C. Dai[a], D. E. Chen[b], K. S. Chen[c], P. K. Tseng[c] and S. Y. Chuang[c]*

[a]National Taiwan Institute of Technology, Taipei, Taiwan, China
[b]Physics Department, Tamkang University, Tamsui, Taiwan, China
[c]Physics Department, National Taiwan University, Taipei, Taiwan, China

A continuous scanning microprocessor-based ACAR system is reported. This system consists of a goniometer and a multiscaler system. The 10-meter long goniometer and its driver and control unit has been reported previously[1]. The multiscaler system consists of four sets of microprocessor-based multiscaler[2]. They register signals from (1) the stationary detector, (2) the moving detector, (3) the coincidence of the two detectors, and (4) the chance coincidence as functions of the position of the moving detector. In order to avoid the position error caused by the backlash in the screw-drive of the moving detector, each set of multiscaler registers two spectra, one for the rightward scan and another for the leftward scan of the moving arm. This system provides simple and reliable measurements for the ACAR experiment.

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*Present address: Department of Physics, University of Texas at Arlington, Box 19059, Arlington, Texas 76019, U.S.A.

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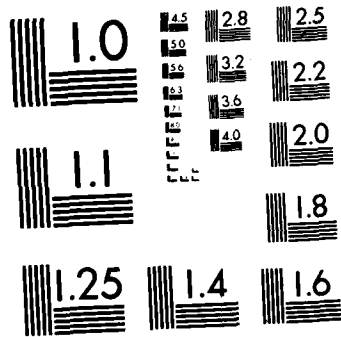
MICROCOPY RESOLUTION TEST CHART

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A LATCHED CONSTANT FRACTION DISCRIMINATOR AND ITS USE
IN TIME RESOLUTION STUDIES

K. Rytsölä
Laboratory of Physics, Helsinki University of Technology
SF-02150 Espoo 15, Finland

A constant fraction discriminator with a latched timing comparator is described. This design improves the temperature stability of the device while providing excellent timing characteristics in a simple construction. An extension of the basic design with upper level discrimination is also presented. The effect of the discriminator adjustments on the time resolution has been measured. The most important adjustment is the input offset of the timing comparator, whose influence on walk characteristics is given explicitly. The time resolution of a complete fast/slow system with these discriminators, RCA C31024 photomultipliers and ϕ 25 mm x 25 mm scintillators is 165 ps when measured with a ^{60}Co gamma source and 50 % energy windows.

The influence of the scintillator on the time resolution has been studied and the resolution is found to depend on the light collection time from the scintillator onto the photocathode, the best shape being a low cylinder or a cone. The best measured resolution, 125 ps, is obtained using ϕ 25 mm x 15 mm cylindrical scintillators with diffusely reflecting surfaces.

Also resolutions with different photomultipliers are compared. Not unexpectedly, the best resolution is obtained with RCA C31024 tubes, but anode pulse amplification, very fast discriminators and care not to distort the pulse shape are necessery to get good results with these tubes.

A POSITRON LIFETIME SPECTROMETER
WITH IMPROVED LINEARITY AND RESOLUTION

Risto Myllylä and Juha Kostamovaara
Department of Electrical Engineering, University of Oulu,
Linnanmaa, SF-90570 Oulu, Finland

A positron lifetime spectrometer is described which consists of improved constant fraction discriminators and a time-to-amplitude convertor. The system is built on two printed circuits mainly with components of MECL III -series. The device is constructed on NIM standard boards.

The comparators of constant fraction discriminators are Plessey's SP9687 ECL-comparators with which better time walk characteristics than with generally used comparators of MECL 10000- and MECL III -series have been achieved.

A special attention has been paid to the linearity of the spectrometer: integral nonlinearity is smaller than ± 0.1 % and differential nonlinearity smaller than ± 2 % in the time range of 30 ns of the spectrometer.

The time resolution (FWHM) of the system is 170 ps by using cylindrical 25 mm x 25 mm NE III scintillators and C31024 photomultipliers with ^{60}Co source and with 30 % side channel windows.

IMPROVED β^+-γ -COINCIDENCE LIFETIME SPECTROMETER

J. Kostamovaara, M. Karras, R. Myllylä
Department of Electrical Engineering, University of Oulu
Linnanmaa, SF-90570 Oulu, Finland

The measuring arrangement consists of a thin slab scintillator which detects positrons penetrating through it and a cylindrical 2" x 2" Pilot U -scintillator which detects annihilation gammas. The source, the β^+ -scintillator, a Pb-absorber and the γ -scintillator are sandwiched for a close geometry.

The positrons which are stopped and annihilated in the β^+ -scintillator contribute the lifetime spectrum with components similar to the source contribution in a conventional lifetime spectrometer. The relative intensities of these components, which depend on the thickness of scintillation material in the positron detector, have been reduced altogether to about 13 % with a 0.5 mm thick positron detector by using a pulse height window of 30 % placed at the β^+ -pulse spectrum. The window eliminates the large pulses due to the captured and scattered positrons. Because a fraction of positrons from the ^{68}Ge source are, however, emitted with an energy too low to penetrate the slab they cause unavoidable signals to trigg the β^+ -channel, and therefore a Pb-absorber has been placed between the β^+ -scintillator and the sample. This arrangement has further reduced the source component to a few percent.

The time resolution is reduced to 340 psec with a 0.5 mm thick Ne104 -scintillator from the previous 250 psec obtained by γ-γ -coincidence method with the 2" x 2" Pilot -scintillators. The efficiency of this method is better than the efficiency of the conventional γ-γ -coincidence method with suitable geometry. Therefore a coincidence rate of several thousands 1/sec is utilized which is important for the quick accumulation of date especially in experiments on the lineshape vs. lifetime dependence.

A DOPPLER-BROADENING LINESHAPE-PARAMETER STANDARD[*]

G. Kögel[‡], L. Smedskjaer[†] and W. Triftshäuser[‡]
‡Hochschule der Bundeswehr München,
8014 Neubiberg, Germany, F.R.
†Materials Science Division, Argonne National Laboratory,
Argonne, Illinois 60439 U.S.A.

The commonly used Doppler-broadening parameters, defined as the ratio between the counts in one or more selected energy regions of the observed spectrum and the total counts in that spectrum, have the advantage of being simple to calculate. They do not, however, have a clear physical interpretation and they are specific to the particular Doppler-broadening equipment used to determine them. Although one might find parameters with a clear physical interpretation (e.g., lifetime) desirable, the instrument specificity is at present the most serious problem, since it makes comparisons between data obtained with different instruments questionable or difficult at best, even when apparently identical definitions of the lineshape parameters have been used.

The present work outlines a simple method by which the instrument specificity can be eliminated, thereby permitting direct comparisons between data obtained with different instruments, provided, of course, that a common definition of the lineshape parameter has been used.

The concept of a generalized lineshape function $G_s(E)$ is introduced as the convolution integral $G_s(E) = N(E)*S(-E) = P(E)*W(-E)$, where $W(E) = R(-E)*S(E)$. In the above expressions, $N(E)$ is the normalized observed spectrum corrected for background, $R(E)$ is the resolution function of the instrument, $P(E)$ is the spectrum one would have obtained for infinite resolution, while $S(E)$ is a weight function. If $S(E)$ is selected as a doublesided step function, then the commonly used lineshape parameters can be obtained as values of G_s for particular arguments E. It will be suggested that rather than basing the definition of a lineshape parameter on the function S, the definition should be based upon a choice of $W(E)$. In doing so, and noting that $R(E)$ is time independent (apart from small instabilities), one may obtain the time-independent and instrument-specific function, $S_W(E)$, as the solution to $W(E) = R(-E)*S_W(E)$. The function $G_W(E)$ can now be calculated from $G_W(E)=N(E)*S_W(-E)$, thereby avoiding a deconvolution for each new spectrum $N(E)$. In this fashion a function $G_W(E)$, which is independent of $R(E)$, is obtained and the instrument specificity has thus been removed. It will tentatively be suggested that for metals the choice $W(E) = \exp[(E-E_0)^2/(2\sigma^2)]$, where $\sigma = 1.00$ keV and $E_0 = 511$ keV, be made. The use of a common definition for all metals, without any special regard to the physical effect being measured, will reduce the sensitivity of this parameter when compared to an optimized lineshape parameter. On the other hand, by using the presently suggested type of parameter, one gains the advantage of being able to compare supposedly identical results obtained with different instruments.

The sensitivity of this new lineshape parameter will be discussed in conjunction with an examination of its statistical properties. Finally a practical example of the derivation and stabilization of the parameter will be given.

THE NEW 2D-ANGULAR CORRELATION APPARATUS
BUILT AT THE UNIVERSITY OF GENEVA

R. Sachot   A.A. Manuel   P.Descouts

Institut de Physique, 24 Quai E.Ansermet

CH - 1211 Genève 4

We describe the components of the 2D angular correlation apparatus developped during the last three years to study solid materials at low temperature :

- The cryogenic system containing the sample, the positron source and a 2T superconducting focusing magnet allows us to measure at 4,2K. Sample heating permit to stabilize the temperature above 4.2K and an optical design control the sample alignment at low temperature.

- The gamma rays detectors are high density proportional chambers . Each detector includes two multiwire chambers and four 1cm thick gamma to electron converters. This solution is a good compromize for time resolution, working stability and fast Compton scattering rejection.
The spatial resolution is 1.1 ± 0.2 mm in both directions, for a sensitive aera of 200 x 200 mm^2. The detector efficiency is $15 \pm 2\%$ for 511 KeV radiation and a time resolution of 300 ± 10 nsec using isobutane.

- The data acquisition is based on the center of gravity method in order to achieve the best angular resolution but with a maximum counting rate of 300 cps. The electronic readout includes 288 independant ADC's triggered by the coincidence logic. A front end microprocessor performs an online data compression and the main computer handle the reduced data to update the 2D angular correlation distribution.

We illustrate the performance of the whole set up with the measurement of the Ps peak in quartz at 4.2K, for a distance of 21 m between the two detectors using 65 mCi of ^{22}Na. The fwhm of the peak is (0.25X0.30) $mrad^2$. This gives a good estimate of the angular resolution of the system.

SCINTILLATION CHARACTERISTICS OF $Bi_4Ge_3O_{12}$ CRYSTALS AS DETECTOR MATERIALS IN A 64 DETECTOR TWO-DIMENSIONAL ANGULAR CORRELATION APPARATUS

H. Iriyama, I. Shinta and S. Tanigawa
Institute of Materials Science, University of Tsukuba,
Sakura-mura, Ibaraki 305, Japan

Positron group at University of Tsukuba is now constructing a 64 detector two-dimensional angular correlation apparatus using $Bi_4Ge_3O_{12}$(BGO) crystals of 20 x 10 x 10 mm and ultracompact photomultiplier tubes (Hamamatsu R647-01) of the diameter of 0.5 inch. In the course of preliminary testing, BGO crystals were found to be very suitable to this apparatus. In the present paper, the scintllation characteristic of crystals are reported. BGO crystals were made by Hitachi Chemical Ltd.. Figures 1 and 2 show typical energy spectra of NaI(Tl) of 13ϕ X 40 mm and BGO crystals for 662 keV γ ray from ^{137}Cs. The peak channel in BGO was found to lie at about 40 % of that in NaI(Tl). This fraction is very large compared with the value 8 % reported previously. In our experimental condition, about 80 % of γ rays are absorbed in both crystals.

Figure 3 shows the optical transmission of BGO crystals. The irradiation of 254 nm ultraviolet photons affected the transmittance of crystals. Figure 4 shows the relation between the absorption coefficient μ and the difference $\mu'- \mu$ after and before irradiation for 70 crystals. From this result, it was found that the crystal with large μ is easily coloured by irradiation. This means the presence of impurity atoms in BGO crystals is very serious. The relation of peak channel with μ was experimentally measured. It was found that easily coulored crystals possess low peak channels. In order to search the effect of impurity atoms the Doppler broadening was measured before and after irradiation in Fig. 5.
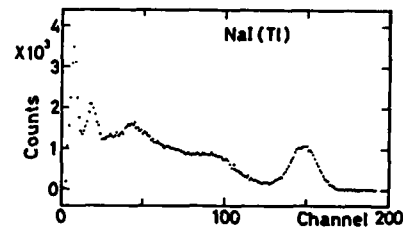
Fig. 1
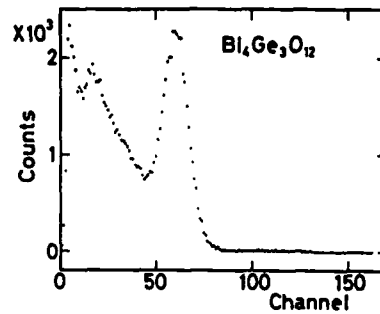
Fig. 3

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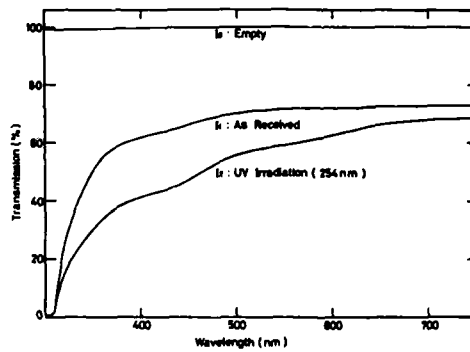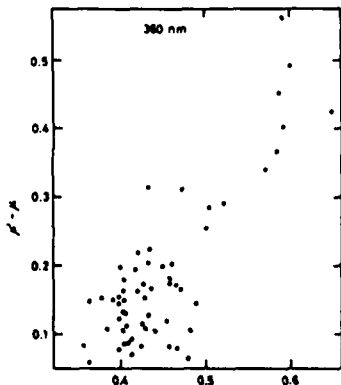
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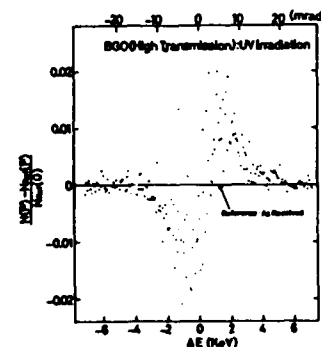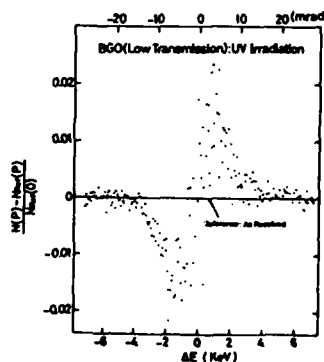
Fig. 5

A SLOW POSITRON ELECTROSTATIC
SYSTEM (SPES) OF NEW DESIGN

A.Dupasquier[a,b] , R.Grisenti[c] , A.Zecca[b,d]
[a]Istituto di Fisica del Politecnico, Milano, Italy
[b]Gruppo Nazionale di Struttura della Materia del CNR, Italy
[c]Istituto per la Ricerca Scientifica e Tecnologica, Trento, Italy
[d]Libera Università di Trento, Povo (Trento), Italy

SPES is a fully electrostatic system, developed for producing a slow-positron beam suitable for surface studies as well as for scattering experiments on gases.

The characteristic features of the system are:

a) complete bakeability for UHV operation;

b) single crystal moderator in backscattering geometry with a ^{58}Co source;

c) a strong retarding lens between the source and the moderator, designed for optimizing the flux of source positrons impinging on the moderator in the energy spectrum region most useful for slow positron production;

d) a spherical energy analyzer of high luminosity;

e) a 1.5 m long beam transport system.

The final positron energy at the target is adjustable from 10 to 10^3 eV (or more, with minor modifications); calculated transmission from moderator to target is 10%; the beam has a diameter of 4 mm and a divergence of 1° at the target in full intensity conditions.

The system is now under testing; experimental data will be presented at the Conference.

THE INFLUENCE OF THE INTEGRATION LIMITS FOR THE DETERMINATION OF LINESHAPE PARAMETERS ON THE EXTRACTED PHYSICAL PARAMETERS.

D.Segers, M.Dorikens and L.Dorikens-Vanpraet

I.N.W., Proeftuinstraat 86, B-9000 Gent, Belgium

Deconvolution of the positron annihilation line is not a very attractive procedure because of the uncertainties in the knowledge of the transfer function of the measuring system and because of the inherently lower resolution of the Dopplerbroadening technique as compared with angular correlation measurements. Therefore Dopplerbroadening of the 511 keV annihilation line is usually characterized by lineshape parameters. Several lineshape parameters have as yet been introduced. One common feature in the calculation of all of them is that a suitable correction for background is necessary. An accurate way to take background effects into account is presented.

The relative effects of temperature in a metal, as measured with lineshape parameters are greatly dependent on the choice of the integration limits for the determination of the desired parameters. In the extreme case where the integration limits are taken very narrow, the effect as a function of temperature will be entirely lost, since the lineshape parameter tends to zero for vanishing width of the window setting. If the intergration limits are taken too wide, the lineshape parameter tends to 1 and again no effect as a function of temperature is seen. In between an ideal choice for the integration limits can be found.

The influence of the width of the central integration window for the definition of the S-parameter on the pre-vacancy effect in indium is discussed. It is demonstrated that the pre-vacancy effect is not an artefact of the integration window settings. From a detailed analysis of the data it is concluded that for a value of the S-parameter close to 0.5 statistically the most reliable results are obtained. The same procedure is applied to the study of pure aluminium in thermal equilibrium and the consequences for the determination of the vacancy formation enthalpy is briefly discussed.

AN INVESTIGATION INTO RADIOSENSITIZER MECHANISMS USING
o-Ps LIFETIME MEASUREMENTS

C.D. Beling and F.A. Smith
Department of Physics, St. Bartholomew's Medical College
Charterhouse Square, London, EC1M 6BQ. U.K.

Radiosensitizers are compounds which are able to enhance the effectiveness of a radiation dose given to anoxic tumour cells, probably as the result of processes which depend on the electron scavenging properties of the compound. In an attempt to investigate the mechanisms involved, we have made o-Ps lifetime measurements in solutions of Duro- and Benzo-quinone in EtOH and Misonidazole in H_2O and EtOH, as a function of concentration and temperature in the range -15 to 80°C.

A three lifetime analysis was used, generally with a fixed free-positron lifetime of 0.39 ns, and the o-Ps yield was corrected to account for the possibility of chemical quenching.

The systems were all found to strongly inhibit and quench Ps. Since the o-Ps lifetime approached the free positron value at high solute concentrations, it was not possible to distinguish clearly between a $(1 + K |M|)^{-1}$ and a $(1 - K |M|)$ concentration dependence of the reduced intensity, and thereby possibly implicate other more complex spur processes. The quenching rate constants are in the order of 10^{10} $M^{-1}s^{-1}$ and indicate the presence of chemical quenching decay channels.

Variation of temperature (Fig. 1) shows that the relative o-Ps yields in the EtOH - based systems increase by only ~10% over the temperature range studied, showing the same dependence as the pure solvent. It is suggested that the solute independence may be explained by the reactivity of radiosensitizers only towards the immediate precursors of Ps (e.g. e^-_{th} and e_t^-). In the water-based system, however, the yield increases initially with temperature but then falls by ~60% as the temperature increases above ~20°C. Since this behaviour is unlike that in pure water, the results can be interpreted on the spur model in terms of the much shorter solvation time and the availability of all the pre-thermal electron states.

The temperature dependence of the quenching rate constants indicates that the o-Ps reactions are diffusion controlled at the lower temperatures, but may show evidence of intrinsic behaviour at the higher temperatures studied.
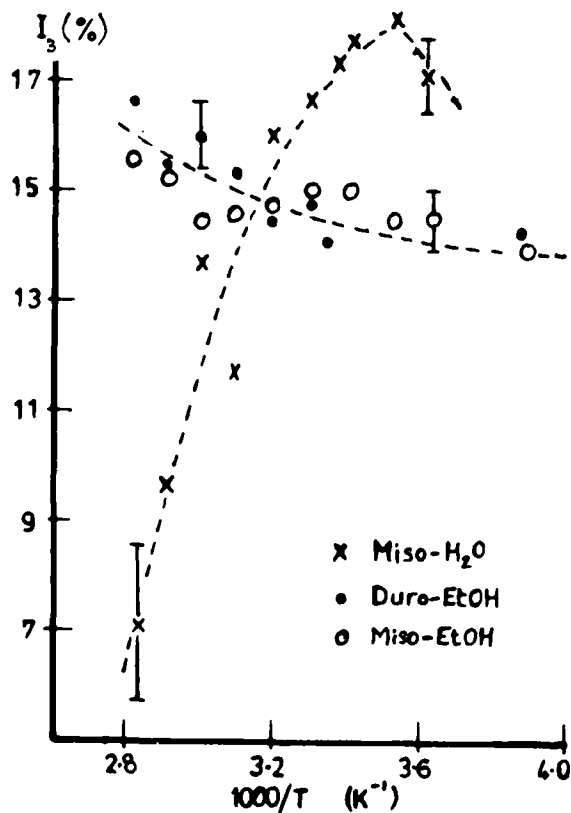
DELAYED COINCIDENCE TECHNIQUES: THEORY AND
EXPERIMENTS FOR A TIME-TO-AMPLITUDE CONVERTER

G.Faraci and A.R.Pennisi

Istituto di Fisica dell'Università di Catania

Gruppo Nazionale di Struttura della Materia-Unità di Catania

Corso Italia 57 - 95129 Catania-Italy

The theory of a widely used delayed coincidence technique,which typically involves a time-to-amplitude converter, has been developed for any intensity of correlated and uncorrelated pulses, arriving at the start and stop channels, taking into account the finite width of the pulses and using poissonian statistical distributions dead-time distorted. Exact expressions have been deduced applying the renewal theory when the distribution of the correlated events is of δ-type. Time spectra have been calculated by means of such a theory in many different situations and checked in two ways: the first using a Montecarlo simulation, the second, performing experimental measurements. Both checks have been found in a very good agreement with the theory.

A SIMPLE METHOD TO STUDY THE REFLECTION AND ABSORPTION OF POSITRONS

S.C. Sharma, J.H. Smith, D.M. Fischer, L.M. Diana, and P.G. Coleman
Center for Positron Studies, Box 19059, UTA Station,
The University of Texas at Arlington, Arlington, Texas 76019, U.S.A.

A simple coincidence technique is described to measure the reflection and absorption of positrons by metals.

The coefficients of reflection for positrons emitted by ^{22}Na have been measured for several samples with atomic numbers in the range 6 - 82.

COEFFICIENTS OF POSITRON MASS ABSORPTION
AND BACK-SCATTERING

P.U.Arifov,A.R.Grupper,H.Alimkulov
Arifov Institute of Electronics,Academy of Sciences Uz.SSR
700052,Tashkent,Observatorskaja,85,USSR

For interpretation of positron annihilation spectra at the uneven distribution of defects within a depth of a sample it is necessary to know the distribution profile of positrons,which can be calculated if the coefficients of positron mass absorption ($m+$) and back-scattering (p^+) are known.

p^+ measurement was made by the following technique.Collimated positron beam directed at a sample located between two scintillometers joined in coincidence scheme. We consider that for a sample with small atomic number Z,polyethylene for example ($Z = 2.4$) the number of registered coincidences is equal to the number of positrons n_o falling at a sample. At increasing of Z of a sample the number of coincidences will be $n_o(I-p^+)$, thus one could determine p^+ using the results of two measurements.

Measurements of p^+ of positrons emitted by Na^{22} and monoenergetic positrons for the production of which a magnetic spectrometer had been used, were made for the samples with $Z =4+82$ (Be,Al, Ti,Ni,Cu,Ge,Mo,Cd,Sn,Ta,W,Pb). The experimental data were appro - ximated by method of least squares. p^+ dependence on Z for non - monoenergetic positrons was approximated by the relation :

$$p^+ = (0.0577 \pm 0.0058) \, z^{(0.4724 \pm 0.0249)} \qquad (I)$$

and for monoenergetic positrons :

$$p^+ = (0.0I94 \pm 0.0047) \, z^{(0.7004 \pm 0.0605)} \qquad (2)$$

moreover eq.(2) was valid for positron energy from I00 to 400 KeV.

Directing the beam of positrons passed through a foil at a sample and registering the decrease of its intensity one could determine m^+ coefficients for different foil materials.However,er rors of such technique, suggested by Takhar /I/, distort m^+ value. Among those one could point out the dependence of efficiency of coincidence spectrometer on beam section of positrons falling on a sample. Positron multiple scattering in a foil leads to the in- crease of beam section and efficiency of coincidence spectrometer decreases. Errors of the technique are due to the fact, that the transformation of energy spectrum of positrons at passing through a foil causes the change of positron back-scattering coefficient. So for p^+ for Cu decreases about I0% at the increasing of foil thickness from 0 to I6.7 mg/cm^2, maintaining it constant at fur - ther increase of thickness till 90 mg/cm^2.

m^+ coefficients for metals may be estimated by measurements of positron lifetime spectra with lesser number of errors.Placing the sandwich of two equal foil samples and positron source (isotope Na) between the polymer plates, e.g. polyethylene, one could determine the fraction of positrons passed through a foil in re- lation of long-time component intensity J of those spectra in such system to the spectrum intensity J registered in a foil absence. For absorbes with $Z=I3+82$,$m+$ dependence on Z is approximated by

$$m^+ = (3I.24 \pm I.09) \, z^{(0.0878 \pm 0.009)} \qquad (3)$$

I.P.S.Takhar,Phys.Rev.,157, 257 (I967).

PROJECTED RANGES OF ELECTRONS AND POSITRONS
WITH ENERGIES BETWEEN 1keV AND 5MeV IN ALL ELEMENTS

H.E. Hansen[1] and U.I. Jensen[2]

[1] Laboratory of Applied Physics II, Technical University of Denmark
Building 307 - DK-2800 Lyngby - Denmark

[2] Physics Laboratory II, Universitetsparken 5
University of Copenhagen - DK-2100 Copenhagen Ø

Penetration of positrons and electrons in elemental random matter was investigated with transporttheory. The influence of elastic scattering off the nuclei was calculated from the Mott series. Using this, rather than for instance the McKinley and Feshbach approximation, enabled us to handle targets with high atomic numbers.

In principle, the employed method allows calculation of any moment of the implantation profile, which might then be constructed from the calculated moments. However, only the first order moment (projected range) and the total pathlength are calculated by the present version of our program.

Calculated values are compared to experimental data and the difficulties of the comparison are discussed together with problems in the theoretical description.

IMPLANTATION AND TRANSMISSION OF POSITRONS IN MOLECULAR SOLIDS AND LIQUIDS UNDER THE INFLUENCE OF HIGH ELECTRIC FIELDS

F. Heinrich and A. Schiltz

Laboratory of Solid State Physics, Swiss Federal Institute of Technology ETH
CH-8093 Zurich, Switzerland

If positrons are injected into organic solids and liquids an electric field $\vec{E}$ parallel to the direction of injection causes three different effects.

(1) During the slowing down period the positron loses its kinetic energy very quickly and also loses the memory of its primary direction. In the presence of a strong electric field the positron picks up energy from the field and is additionally forced into the direction of $\vec{E}$. Thus, the linear absorption coefficient μ becomes dependent on $\vec{E}$.

(2) During the diffusion period the thermalized positron performs a drift motion with velocity $v_+ = b_+ E$, where b_+ = mobility.

(3) If the material is a non-polar dielectricum the probability for Ps-formation is altered by the field. The latter effect is independent of the field direction.

Implantation experiments are a suitable tool to measure the annihilation probability at a certain depth x within the sample. The relative change of the counting rate $\Delta N/N = \left[N_E(x) - N_0(x) \right] /N_0(x)$ (E, 0 = field on, off, respectively) is sensitive to the effects (1) and (2) if the single-counting rate is measured and additionally to (3) if the annihilation quanta are counted in coincidence.

In the single-rate mode, $\Delta N/N$ turns out to be linearly dependent on $\vec{E}$. The x-dependence is parabolic with a positive/negative slope for $\vec{E}$ accelerating/decelerating, respectively. The parabolae for positive and negative field polarity are strictly symmetric with respect to the x-axis. In the coincidence mode, however, a pronounced asymmetry observed in non-polar materials indicates the $\vec{E}^2$-dependent variation of the peakrate due to the field dependence of the Ps-formation.

Unfortunately, a separation of the effects (1) and (2) is not possible in the course of implantation experiments. Thus, as an additional experiment, the $\vec{E}$-dependence of the positron transmission was measured in polyethylene, polypropylene and polymethylmetacrylate (polar). The following relation between the linear absorption coefficient μ_E ($\vec{E}$ on) and μ_0 ($\vec{E}$ off) applies:

$$(\mu_E - \mu_0) / \mu_0 = - E\, a\, (1 + c\mu_0 x)$$

The constants a and c are positive and quite similar for the different materials. Using this relation we calculated the slowing-down contribution [effect (1)] in the implantation measurements and compared it with the experimental data. For single rate measurements the difference is simply the drift contribution $(\Delta N/N)_{drift} \sim v_+ \tau_{bulk}$. For the polymers mentioned above, the e^+-mobility turns out to be extremely small, $b_+ \leq 0.3$ cm^2/Vs, whereas in n-hexan a field-independent mobility $b_+ = (60 \pm 20)$ cm^2/Vs was found for fields up to 150 kV/cm.

From the same experiments the field dependence of the positronium formation in n-hexan and other organic liquids can be deduced up to a field strength of 150 kV/cm.

CONTINUOUS SLOWING DOWN APPROXIMATION OF 50 KeV -100 MeV POSITRONS

S.K. Gupta and D.K. Gupta
Department of Physics, S.V. College,
Aligarh (Agra University)
India

The Wilson theory has been modified for the calculation of the continuous slowing down approximation(csda) range of 50keV-100 MeV positrons in the absorbers of atomic numbers from 1 to 92 and in some detector materials, minerals, organic compounds. A correction factor which depends on energy as well as on atomic number is evaluated. Values of csda range obtained by the present approach have shown an agreement with theoretical values within a discrepancy of 6-7%.

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POSITRON DIFFUSION IN GERMANIUM[1]

H. H. Jorch[+], K. G. Lynn, I. K. MacKenzie[*]

Brookhaven National Laboratory, Upton, N.Y. 11973 USA
+ presently at Chalk River Nuclear Laboratories, Chalk River
Ontario K0J 1J0 Canada
* University of Guelph, Guelph, Ontario N1G 2W1 Canada

The temperature dependence of the diffusion length of positrons (L_+) has been investigated in Ge. Monoenergetic positrons from a slow-positron beam[2] are implanted at various energies, and the energy spectrum of annihilation events is used to obtain the fraction of positrons which diffuse to the surface and form positronium.[3] A one-dimensional diffusion model[4] is used to derive the positron diffusion length. The results indicate a strong motion-limiting mechanism, with onset above room temperature (~ 500 K) and saturation well below T_m (~ 900 K). Unlike the situation in similar experiments conducted with metal specimens, this decrease of L_+ cannot be accounted for by trapping at thermally generated vacancies. An interpretation in terms of a two-state model involving high-temperature lattice dilatation trapping into a polaron-like state is proposed.

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ENERGY LOSS SPECTRA OF POSITRONS
SCATTERED FROM SOLID SURFACES*

J. M. Dale, L. D. Hulett
Analytical Chemistry Division, Box X
Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830, U.S.A.
S. Pendyala
Department of Physics
State University of New York, College at Fredonia
Fredonia, New York 14063, U.S.A.

Several groups have been successful in producing usable intensities of mono-energetic low-energy positron beams in the last few years (1-4). This has led to attempts to investigate positron spectroscopies which pattern the various electron spectroscopies currently being used. Positron spectroscopies of solids and solids surfaces are of special interest and the first measurements of low-energy positron diffraction (LEPD) from a single crystal surface have been reported (5).

The authors have reported the first experimental measurements of positron energy losses from solid surfaces.(6) Because secondary electrons or positrons can be alternately ejected from the low-energy positron gun, depending on the bias potentials, we were able to compare the spectra of positrons and electrons scattered from the same surfaces under identical scattering geometries. Surfaces of tungsten and silicon were bombarded with monoenergetic beams of positrons and electrons and spectra were recorded for shallow scattering angles with respect to the incoming beam. Discrete energy loss peaks were observed for both positrons and electrons at kinetic energies about 15 eV lower than that of the elastic peaks. For higher energy losses the positron spectra were significantly different from the electron spectra. Possible interpretations of the energy loss spectra for tungsten and silicon involve low-momentum interband transitions, plasmon losses and losses from core electron ionization.

Positron energy loss studies are being continued for other solid surfaces as well as for tungsten and silicon under improved experimental conditions. Current results will be presented.

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DIRECT OBSERVATION OF POSITRONIUM STATES AT THE SURFACE OF ULTRAFINE PARTICLES AND THE INTERNAL SURFACE (VOIDS) BY POSITRON AGE-MOMENTUM CORRELATION

Y. Kishimoto[#], S. Tanigawa[#], H. Morinaga[##] and Y. Matsuoka[##]

#)Institute of Materials Science, University of Tsukuba,
Sakura-mura, Ibaraki 305, Japan
##)Department of Physics, Meijo University,
Tenpaku-ku, Nagoya 468, Japan

Correlation measurements between positron age and momentum distribution of annihilation pairs were carried out in ultrafine particles of some metals. Figures 1, 2, 3 and 4 show the results of nickel of mean diameters 100 A, 300 A and 1000 A, and gold of mean diameter 250 A.   All of them were obtained at room temperature in air.   The momentum dependence of mean lifetimes (τ_M) shows the same tendency in each sample.   This characteristic change of τ_M is understood by coexistence of para positronium and ortho-para conversion process.   Furthermore, it was suggested that the momentum distribution of positroniums passing through the conversion process is narrower than usual self annihilation process.   The results of nickel 100 A and 300 A and gold of 250 A can be overlapped each other when they are slightly shifted.   It has been considered that the surface of gold is free from oxidation or absorption of gas molecules.   Therefore, it seems that positron or positronium is little affected by oxide layer.   The change of mean lifetimes in nickel 1000 A was larger than the case of 100 A and 300 A.   This means the decrease of the number of sites for surface trapping with the increase of particle size.   It is worth to point out here the following fact.   The momentum dependence of lifetimes observed in ultrafine particles qualitatively corresponds to the results of neutron irradiated molybdenum by Mackenzie et al. This fact is a clear experimental evidence that the internal surface (voids) is the same as the external surface in the point of view of positron annihilation. Experiments on voids in molybdenum and aluminum are now in progress.
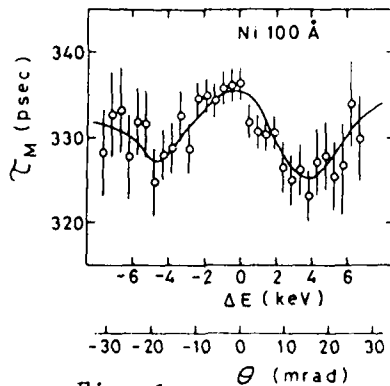
Fig. 4

Fig. 1
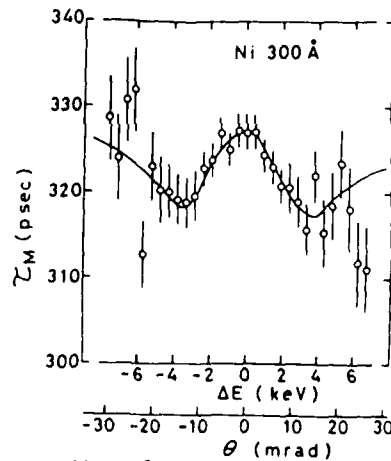
Fig. 2
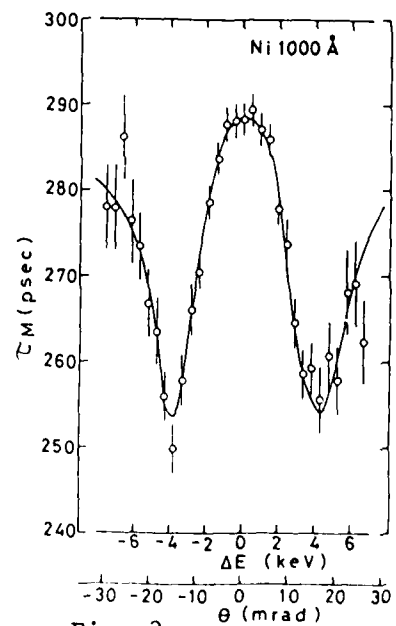
Fig. 3
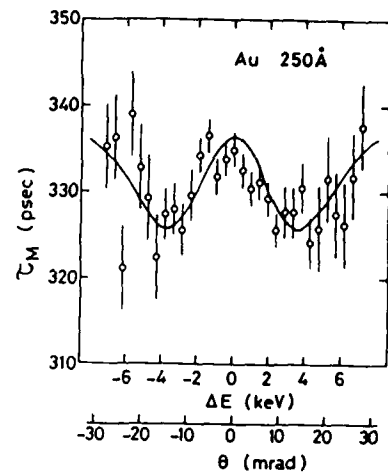
PROGRESS ON MEASUREMENT OF POSITRON SURFACE-STATE LIFETIMES

Allen P. Mills, Jr.

Bell Laboratories, 600 Mountain Avenue, Murray Hill, NJ 07974 USA

An attempt is being made to measure the lifetime of positrons bound in their "image-potential" well at the surface of a metal. This interesting parameter has been calculated[1] using several different models; a comparison with experiment would test our understanding of correlation effects and the non-adiabatic nature of the "potential".

The measurement uses a slow positron beam bunched[2] into sub-nanosecond length bursts with no "start" counter needed. The "stop" counter which signals the positron decay is a Hamamatsu R1294UX + Pilot U which works well in the ~150G ambient magnetic field. The preliminary measurement shown in the figure, although plagued by stray positrons that give a pedestal to the 0.8 nsec FWHM time resolution, allow us to estimate crudely the surface state lifetime τ_s for a Cu(100) + S surface. With the sample at 900K, only a small fraction of the positrons annihilate from the surface state because they are thermally desorbed[3] as positronium at a high rate. Except for annihilation from a few positrons which strike a grid or decay in the bulk crystal, one expects a single lifetime $\tau = 125$ psec from $^1S_0$ positronium with $I \approx 25\%$. The ~500 psec slope in the figure seems to indicate that the time resolution curve has a slope of ~375 psec. The room temperature time distribution shows a ~750 psec lifetime which we correct to ~375 psec by subtracting off the time resolution slope. This agrees roughly with the expected room temperature time distribution: $\tau_1 = 125$ psec, $I_1 \approx 12.5\%$ for $^1S_0$ positronium, and $\tau_s \approx 500$ psec, $I_s \approx 50\%$ for the surface state. It is hoped that there will be improved data to present at the conference.
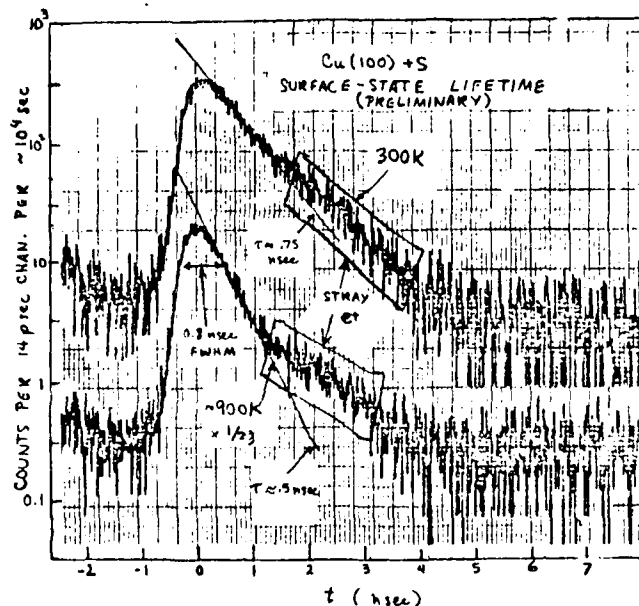
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ELECTRON AND POSITRON WORK FUNCTIONS OF Cr(100)

R. J. Wilson and A. P. Mills, Jr.
Bell Laboratories, Murray Hill, NJ 07974, U.S.A.

We report measurements of the electron and positron workfunctions of clean single crystal surfaces of Cr(100) in ultra high vacuum. The positron work function ϕ_+ is obtained by measuring the spectrum of slow positrons re-emitted by the Cr(100) surface when it is bombarded with keV energy positrons[1]. The electron work function ϕ_- is measured relative to Al(100) by comparing the target biases at which the slowest emitted positrons are recollected by the target. We obtain ϕ_+=-1.76(5) eV and ϕ_-=4.46(6) eV for Cr(100) using the value ϕ_-=4.41(3) eV for Al(100) reported by Grepstad, Gartland and Slagsvold[2]. The ϕ_+ value is in agreement with the -2.2 eV calculated by Nieminen and Hodges[3]. The positronium work functions for Cr implied by these results are -4.10(4) eV eV and + 1.00(5) eV for the n=1 and n=2 states respectively; the positronium negative ion[4] (Ps$^-$) work function for Cr is calculated to be -0.01(7) eV. A search for Ps$^-$ showed that at a 90% confidence level less than one positron in 10^3 thermalized positrons reaching the Cr surface are emitted as Ps$^-$.

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A METHOD FOR CALCULATING POSITRON
WORK FUNCTIONS OF SOLIDS*

J.L. Fry and P.C. Pattnaik
Department of Physics, Box 19059
The University of Texas at Arlington, Arlington, Texas 76019, U.S.A.

A method for the consistent evaluation of positron work functions in solids is presented and applied to chromium. The method is based upon the availability of both experimental work functions and self-consistent-field band calculations for electrons. These may be used to construct a periodic potential for a positron moving in an infinite solid and to remove the non-uniqueness of the additive constant in the potential. The nature and origin of this non-unique constant for the infinite solid is discussed in detail. Including a correlation correction, the computed positron work function for chromium is -2.78 eV compared with the experimental value of -1.76±0.05 for a Cr(100) surface.

POSITRON STIMULATED SECONDARY ELECTRON EMISSION FROM A Cu(100) SURFACE[*]

Alex H. Weiss and Karl F. Canter
Physics Department, Brandeis University
Waltham, Massachusetts 02254, U.S.A.

An electrostatically guided monochromatic slow (40-400 eV) positron beam[1] was used to produce secondary electrons by bombardment of a clean copper (100) surface (characterized by Auger electron spectroscopy) under ultra high vacuum conditions. The results of measurements of positron induced secondary electrons are compared with measurements of secondaries produced by an electron beam using the same optics and impinging on the same sample. Comparisons are also made with previous positron[2,3] and electron[4] work.

Secondary electrons were detected using a channel electron multiplier mounted behind a retarding field analyser (RFA) on a moveable arm.[1] Measurements were made of the angular distribution ($dN/d\Omega$) of both positron and electron stimulated secondary electrons at several incident beam energies ranging from 40 eV to 400 eV. Both positrons and electron distributions were found to vary approximately as $\cos(\theta)$ (where θ is measured relative to the crystal normal). This distribution is similar to distribution found previously for electron stimulated secondaries.[4]

The angular distributions were integrated over 2π solid angle and divided by the incident beam flux to obtain the total secondary yield per incident particle, δ, which we found to be 0.97 $\pm$ 0.20 for positrons and 1.05 $\pm$ 0.20 for electrons at 400 eV. This compares with δ = 1.3 for electrons incident on copper at 600 eV tabulated by Dekker.[4] The ratio of electron to positron secondary yield obtained from our data, 1.0 $\pm$ 0.3 at 400 eV is consistent with the results of Pendyala and McGowan[3] who measured a ratio of 1.2-1 with a primary beam of energy 100-1000 eV incident on a lead glass channel electron multiplier. We differ from the results of Cherry[2] who in his pioneering slow positron work obtained a ratio of 3.0 $\pm$ 0.3 from an oxidized Mg-Ag alloy.

In addition to angular distributions we measured the energy distributions of secondaries from both e^+ and e^- bombardment for fixed primary beam energy and angle using the RFA. We also measured the yield of secondary electrons for fixed angle as a function of primary e^+ and e^- beam energies.

In all of the above measurements the positron results were found to be similar to both the electron results obtained in our systems and to electron results obtained in work by others.[4] This finding is consistent with theoretical models of secondary emission[4] and the assumption that the penetration depth and the rate and nature of energy loss of the primary positron or electron beam is the same for energies above 100 eV.

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THE FRACTION OF RE-EMITTED POSITRONS AND
OF THE POSITRON WORK FUNCTION FOR Cu(111)+S BETWEEN 50 AND 350K*

P. J. Schultz and K. G. Lynn
Brookhaven National Laboratory
Physics Department
Upton, New York 11973, U.S.A.

A beam of 1 keV positrons incident on a Cu(111)+S surface has been used to study the dependence on temperature (50 to 350 K) of the positron work function (ϕ_+) and the yield of re-emitted positrons. A positive dependence of the slow-positron yield on temperature is found which is attributed in part to the reduction in the magnitude of ϕ_+ ($\sim$25%) at 50 K relative to its value at 300 K. In addition, evidence will be presented for a decrease in the positron-phonon scattering at the metal-vacuum interface at low sample temperatures. At lower sample temperatures a large decrease in the yield has been predicted by the model of a plane-wave positron incident on a one-dimensional attractive step[1] (i.e. sample surface). The data do not show the magnitude of decrease at the lower temperatures that would be predicted by this model. A possible explanation for this disagreement is that the 1 keV positrons are not fully thermalized before reaching the sample surface and escaping into the vacuum.

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POSITRON ANNIHILATION IN THE BULK AND ON THE SURFACE
OF Cu - Zr AMORPHOUS ALLOYS

I.Ya.Dekhtyar, Ch.Abraev, E.G.Madatova, M.M.Nischenko
Institute of Metal Physics, Acad.Sci.UkrSSR, Kiev-142, USSR

The method of electron-positron annihilation (EPA) was used to investigate electron states in the bulk and on the surface of $Cu_{60}Zr_{40}$ alloys with iron additions. Angular distribution of annihilation photons (ADAP) on the surface was obtained with the use of positronium atoms produced in the convertor from Si single crystals. The transition from crystalline into amorphous state is accompanied by electronic structure changes in the bulk and on the surface. The fact that EPA characteristics vary on the surface at the transition into amorphous state is explained in terms of two factors: the charge transfer and the adsorbtive change in the surface layer composition. Addition of Fe into the alloy alters drastically the EPA characteristics at the transition to the amorphous state this being true for both the bulk and the surface. But the concentration of conduction electrons in the bulk and on the surface remains unchanged during this transition. The scheme in the figure shows that the prevailing localization of positrons on the atoms of this or that species in the bulk and on the surface of Cu $_{60}Zr_{40}$ alloy varies at the transition from crystalline to the amorphous state.
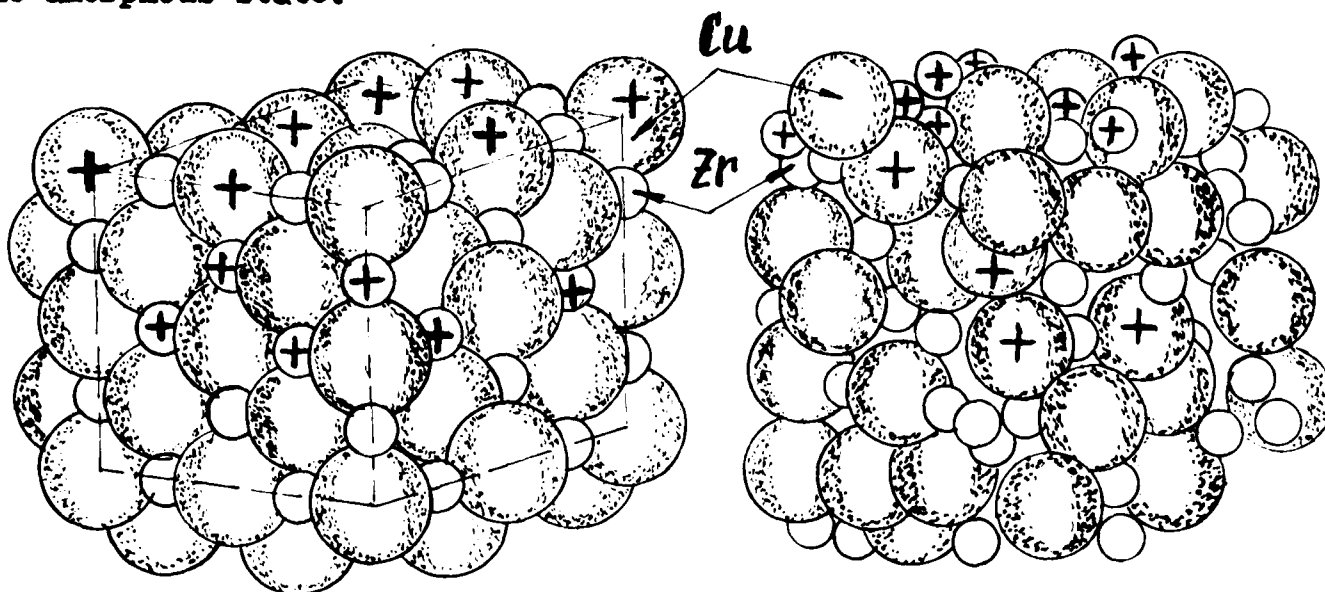
POSITRON ANNIHILATION ON THE SURFACE OF MOLIBDENUM SINGLE CRYSTALS

I.Ya.Dekhtyar, V.I.Silant'ev, S.G.Sakharova, V.I.Patoka, S.Yu.Mityagin

Institute of Metal Physics, Acad.Sci.UkrSSR, Kiev-142,USSR

Electronic structure of Mo (IOO) surface was investigated using the method of positron convertion into positronium atoms (Ps). Angular distribution of annihilation photons (ADAP) differs essentially from that in the bulk. ADAPs obtained from accurately prepared Mo (IOO) surface in the ultrahigh vacuum contain beside Ps also a fine structure whose position depends on the interaction between the surface and residual gases. ADAP's complex structure is explained as a superposition of contributions from corresponding electronic groups which are characterized by relevant limiting values of electronic momenta. ADAP from the surface in the ultrahigh vacuum indicates the presence of at least four groups of conduction electrons and two groups of core electrons. The results correlate with calculated local density of electron states for Mo (IOO).

The effect of small additions of carbon and oxygen on the annihilation characteristics of the Mo (IOO) was studied under real conditions. Essential modifications in the surface electronic structure may be infered from the obtained results. It is shown that electronicstructural characteristics of metal surface obtained by the method of positron annihilation make it possible to define in principle also such electronic properties as the metal surface tension.

OBSERVATION OF SLOW POSITRON REFLECTION FROM LiF

P.G. Coleman, D.R. Cook, S.F. Schaffner, L.M. Diana, S.C. Sharma, and S.Y. Chuang
Center for Positron Studies, Box 19059, UTA Station,
The University of Texas at Arlington, Arlington, Texas 76019, U.S.A.

A simple time-of-flight spectrometer has been used to measure the intensity of a specularly-reflected slow positron beam from a crystal surface as a function of incident positron energy.

The slow positron source consists of a 120 microcurie ^{22}Na deposit covered with a thin disk of fast plastic scintillator, positioned 1.5mm behind a moderator assembly consisting of vanes of annealed tungsten ribbon. About 20 slow positrons per second, in a 1cm - diameter beam, are guided by simple electrostatic lenses to the surface of a LiF crystal (cleaved in the 100 plane) held 10cm away at 45° to the incident beam direction. A channel electron multiplier (CEM) is positioned 4cm from the crystal, along a direction at 90° to the incident beam, so that any reflected positrons are collected and timed from source to crystal to detector. The apparatus is housed in a small stainless steel vacuum system pumped by a 30l/s diode ion pump and surrounded by magnetic shielding. The time-of-flight technique makes possible measurements at very low beam intensities (rates as low as 0.01 sec^{-1} have been measured).

Strong peaks in the reflected beam intensity were observed at 14 and 22 eV, with a third, smaller peak at 53 eV. The two prominent peaks merged into one, centered at 16 eV, after a time lapse of three months, indicating a change in the surface condition. No special procedures were followed with regard to preparation and maintenance of surface cleanliness; the freshly-cleaved crystal was installed immediately into the system, which was baked for twelve hours prior to taking the first measurements.

The incident beam intensity was seen to increase smoothly from 2 sec^{-1} to an asymptotic level of 20 sec^{-1} between 5 and 150eV, measured by moving the CEM to an in-line position. The reflected intensities observed were as high as 0.15% of that of the incident beam at the strong low-energy peaks, falling to under 0.01% at 100eV and above.

These preliminary results demonstrate the feasibility of time-of-flight surface studies and further measurements will be made with apparatus of improved design.

APPLICATION OF POSITRON AGE-MOMENTUM CORRELATION MEASUREMENTS
TO THE STUDY OF DEFECTS IN INORGANIC MATERIALS

S. Tanigawa[#], Y. Kishimoto[#] and N. Tsuda[##]
#)Institute of Materials Science, University of Tsukuba,
Sakura-mura, Ibaraki 305, Japan
##)National Institute for Researches in Inorganic Materials,
Sakura-mura, Ibaraki 305, Japan

Positron technique has been successfully applied to the study of defects in metals. In non-metallic materials, however, the study of defects by this technique has not yet been established due to the complicated annihilation modes of positrons in them. In the present work, we developed a high counting rate measurements of positron age-momentum correlation using a fast-fast timing system and applied to non-metallic materials containing defects. Triple coincidence rate of the system was about 50 cps. In the past experiments at University of Guelph and at University of Tokyo, it was 1 $\sim$ 3 cps. Figure 1 shows the resolved lifetime as a function of momentum in NaCl crystal exposed to ^{22}Na source of 50 µCi for a couple of months. This result is quite different from that in X-ray irradiated crystal shown in Fig. 2. Figure 3 shows the results of MgO single crystals containing dislocation densities of 10^4 and 8.7 X 10^7 cm^{-2}, respectively. Figure 4 shows the results of Al$_2$O$_3$ single crystals containing dislocation densities of 3.7 X 10^5 and 2.7 X 10^8 cm^{-2}, respectively. Figure 5 shows the results in sintered BaTiO$_3$ polycrystals with stoichiometric and nonstoichiometric compositions. The dependence of lifetime in MgO, Al$_2$O$_3$ and BaTiO$_3$ on momentum are quite different from the case of NaCl crystals. This difference is due to the presence of positroniums in NaCl. In other crystals, positrons interact with defects as the positron states other than positroniums.
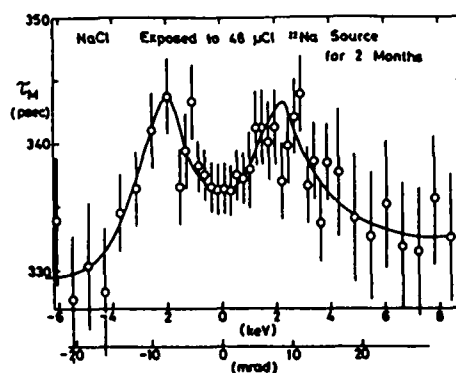
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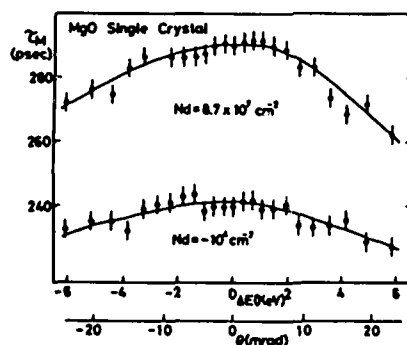
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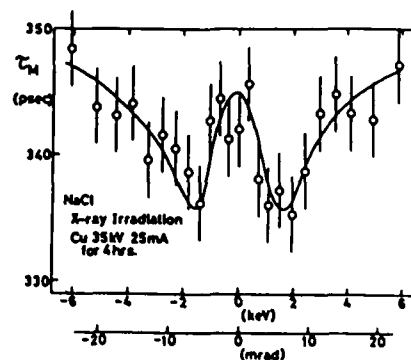
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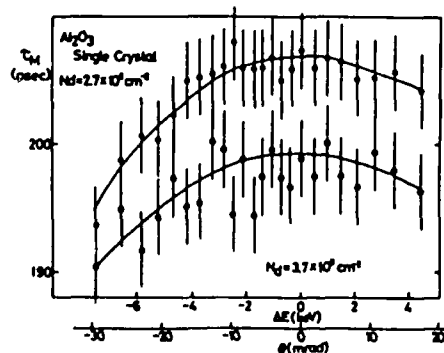
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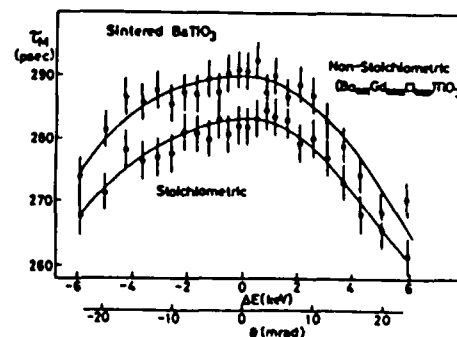
Fig. 5

LIFETIMES IN SOLID ARGON WITH HIGH VACANCY CONCENTRATION[a]

D. M. Schrader, A. Loewenschuss[b], J. Y. Jean[c], K. Nakamoto,
B. D. Pollard, and R. E. Svetic
Chemistry Department
Marquette University
Milwaukee, WI 53233, U.S.A.

Gaseous argon is sprayed onto a cold (10K) copper surface on which 10μCi Na^{22}Cl had been previously deposited. The argon matrix thus formed is believed to contain a high concentration of vacancies, but these have not been well characterized[1]. After subtracting $\sim$50% correction for annihilation in copper, the argon lifetime spectrum is analyzed into three components, two corresponding to positronium (47%, 3.2ns and 16%, 0.12ns) and one to positrons (37%, 0.22ns). Isochronal annealing up to 50K (the maximum temperature attainable with our apparatus) reduces the o-Ps component intensity and lifetime to 23% and 2.5ns, while at the same time increasing the positron component intensity and lifetime to 69% and 0.39ns. These appear to be approaching the 84K values for o-Ps(10%, 2.2ns) and positrons (86%, 0.40ns) reported by Haberl[2]. The four linear plots of our o-Ps and e$^+$ lifetimes and intensities vs. annealing temperature are superimposable on one temperature scale. These observations suggest that one vacancy type is responsible for (a) trapping positrons, as well as (b) forming and trapping positronium. An estimate of the mean size of this vacancy is possible.

Simultaneous positron lifetime measurements and resonance Raman spectra with NO$_2$ doped argon matrices were also performed.

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POSITRON ANNIHILATION IN SOME BARIUM BORATE GLASSES CONTAINING TRANSITION METAL OXIDES

[†]S.G. Usmar[*] and H. Rawson
University of Sheffield, Sheffield, England

and

R.N. West
University of East Anglia, Norwich, England

Results of positron lifetime and angular correlation measurements for the glass series $xM_sO_r:(1-x)(0.4BaO:0.6B_2O_3)$ are presented ($M_sO_r \equiv V_2O_5; Fe_2O_3$ and CuO). All glasses exhibit two or three component lifetime spectra, $\tau_1 \approx 200ps$; $\tau_2 \approx 300\text{-}400ps$ and $\tau_3 \approx 800ps$. τ_1 is attributed to a mixture of pPs and bulk state annihilation; τ_2 to a trapped or bound state and τ_3 to oPs pick-off. Supporting evidence for these assignments is found in the angular correlation results.

[*]Present address: Case Western Reserve Univeristy, Cleveland, Ohio 44106 U.S.A.

[†]Work completed in partial fullfilment of Phd.

THREE - QUANTUM ANNIHILATION IN GAMMA - IRRADIATED TEFLON.

C. Dauwe *,**   and Motoko Kwete *

  * ; Universite Nationale du Zaire, Campus de Kinshasa, B.P. 190
      Kinshasa XI, Republique du Zaire.
 ** ; Laboratorium voor Magnetisme, Rijksuniversiteit Gent,
      Proeftuinstraat 86, B-9000 Gent, Belgium.

Recent lifetime experiments by Kindl et Al.(1) on gamma - irradiated
teflon (Polytetrafluoroethylene) have been resolved into four unres-
tricted components. In accordance with D.P.Kerr (2), only the longest
lived component $T4 \sim 4$ ns has been attributed to the forced two quan-
tum decay of an orthopositronium(O-Ps) state, whereas the three other
components are considered to belong to free positrons ($T2 \sim 0.38$ ns),
trapped positrons ($T3 \sim 1.4$ ns), and eventually parapositronium decay.
($T1 \sim 0.12$ ns).
From these lifetime parameters the absolute three quantum yield P can
be calculated under different assignements for the components and
these values can be compared to experimentally obtained three-quantum
yields, according to the relation;

$$P = \frac{1}{372} \left(1 - \frac{4}{3} \sum \frac{T0 \times Ii}{T0 - Ti} \right) + \sum \frac{Ii \times Ti}{T0 - Ti} \qquad (a)$$

Where the index i indicates all the components related to O-Ps decay,
and T0 is the natural O-Ps decay mean lifetime ~ 136 ns. We have used
our three -detector orthopositronium spectrometer described elsewhere
(3) to measure accurately the three quantum yield P in freshly quen-
ched teflon, and in a series of samples irradiated in a Cs-137 source
up to 14 Mrad total dose. Correction for compton scattering of the
annihilation radiation, and for partial escape of the positrons where
taken into account. Our experimental results agree with the Kindl re-
sults for all doses only if both T3 and T4 are taken into account in
form. (a).
As a result it seems that both T3 and T4 are O-Ps related, and that
the Kerr/Kindl assignement might be subject to discussion.

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STUDY OF d-ORBITAL PARTICIPATION IN BONDING BY POSITRON LIFETIME TECHNIQUE

V. Manohar, S. Ramasamy and T. Nagarajan[+]
Department of Nuclear Physics, University of Madras,
A.C.College Campus, Madras 600 025, India.

In an earlier paper Ramasamy et al.[1] have discussed their positron angular correlation results in organic compounds viz., m- and p-nitroaniline (I and II), m- and p-methylsulphonyl -N, N-dimethyl aniline (III and IV), p-phenoxyaniline (V) and p-phenylthioaniline (VI) to investigate the involvement of the d-orbital of sulphur in bonding. They have concluded that the d-orbital of sulphur is involved in bonding in compound IV and ligand perturbation is necessary for d-orbital contraction. In this paper we report positron lifetime measurements on these samples to further investigate the d-orbital participation in bonding and to see whether there is any positronium (Ps)formation. Three component fit has been made in all these samples using POSITRONFIT[2] program. The compounds I and II were chosen to see the effect of conventional resonance phenomenon on positron lifetime. The probability of Ps formation in these samples becomes very small due to the high dipole moments with excess electron density at the oxygen site[3].The intensity of the third component in the p- and m-isomers is 2.8% and 0.5% respectively. The intensity of the second component I_2 decreases by 10% in the paranitroaniline. However this does not produce an appreciable change in the angular correlation curve[1]. In the case of compounds III, IV, V and VI, T_3 remains almost the same (T_3 =1.1nsec) and the intensities are 34%, 24%, 24%, 24% respectively. The value of I_3 for compounds V and VI is constant, but it decreases for compound IV compared with III. In addition there is an increases of I_2 to 50% for compound IV compared with 35% for compound III. One should note that in the case of p-nitroaniline I_2 decreases relative to the meta isomer whereas in the case of the p-methylsulphonyl-N, N-dimethylaniline I_2 increases relative to the meta isomer. This reverse trend in I_2 and the decrease in I_3 are explained as due to the participation of the d-orbital of sulphur in bonding in compound IV.

[+]Present Address: Foster Radiation Laboratory, McGill University,
Montreal, Canada.

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POSITRON LIFETIME MEASUREMENTS IN Pb^{2+} DOPED KCl SINGLE CRYSTALS

M. Chinnusamy, S. Ramasamy, V. Manohar and T. Nagarajan[+]
Department of Nuclear Physics, University of Madras,
A.C. College Campus, Madras 600 025, India.

Positron lifetime measurements were carried out in pure KCl and in that doped with Pb^{2+} impurity to concentrations of 100 ppm, 550 ppm and 1050 ppm. All lifetime spectra were analysed with three components, using the program POSITRON FIT[1] and the parameters are given in the table below.

Sample	T_1	T_2 (psecs)	T_3	I_1	I_2	I_3	k_2	k_3
Pure KCl	159±6	427±19	722±23	34±2	46±2	20±3	1.80	1.00
KCl+Pb 100 ppm	147±7	444±16	778±19	30±1	46±2	24±3	2.08	1.29
KCl+Pb 550 ppm	148±7	419±25	708±17	32±2	40±2	28±3	1.72	1.51
KCl+Pb 1050 ppm	147±6	442±13	761±23	25±1	57±2	18±3	2.59	1.02

All the three lifetime components T_1, T_2 and T_3 are almost constant in pure, Pb^{2+} impurity doped KCl crystals, whose values are about 150, 450 and 750 psecs respectively. The intensity I_1 of the first component remains more or less the same upto 550 ppm impurity concentration, with a light decrease for 1050 ppm impurity concentration. The intensity I_2 of the second component decreases in 550 ppm impurity concentration and considerably increases in the higher impurity concentration of 1050 ppm. Following Brandt et al.[2], the positron capture rates k_2 and k_3 are calculated using the relations $k_2 = I_2 (\frac{1}{T_1} - \frac{1}{T_2})$ and $k_3 = I_3 (\frac{1}{T_1} - \frac{1}{T_3})$. A considerable decrease in k_3 and at the same time considerable increase in k_2 in the case of 1050 ppm impurity concentration implies possible precipitation of impurities.

[+]Present address: Post Radiation Laboratory, McGill University,
            3610 University Street, Montreal I.J.
            Canada H3A 2T2

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STUDY OF OPTICAL STIMULATION OF THE ELECTRON-POSITRON ANNIHILATION IN IONIC CRYSTALS

P. Topalov and T. Troev*
Physics Department of the Sofia University, Sofia-1126, Bulgaria
*Institute of Nuclear Research and Nuclear Energy,
Sofia-1184, Bulgaria

The idea of the experimental method suggested in the present paper is to stimulate the annihilation of the positrons in the ortho-quasipositronium state with the help of an intensive soft-photon beam. The electron-positron annihilation in the ortho-quasipositronium states in ionic crystal will be mainly discussed here, because the explanation of the experimental method essence is easy to be carried out for these crystals.

The dependence of the measurable quantities on the medium parameters, on the spectral and spatial distribution of the stimulating laser beam, on the experimental geometry and others is investigated. A comparison with a similar experimental method is performed.

The basic theoretical expressions in this paper are:

$$\sigma_1 = \frac{3}{2} \cdot \frac{K_{12}}{\lambda_1^{sp} + \frac{1}{4} K_{12}} \cdot \frac{1.8 \, arctg \frac{1}{2} \frac{nc^3}{A \cdot w_0^2 \cdot w_L} \cdot n(\Delta w_L)}{1.8 \, arctg \frac{1}{2} \frac{nc^3}{A w_0^2 w_L} \cdot n(\Delta w_L) + 1} \cdot \frac{\theta}{\Delta\sigma}$$

$$\sigma_2 = 1.8 \, arctg \frac{1}{2} \frac{nc^3}{A w_0^2 w_L} \cdot n(\Delta w_L) \Big/ \Big[1.8 \, arctg \frac{1}{2} \cdot \frac{nc^3}{A w_0^2 w_L} \cdot n(\Delta w_L + 1 \Big]$$

The coefficient σ_1 is a measure of the spatial anisotropy of the annihilation radiation in the sample in the presence of a stimulating laser radiation. The coefficient σ_2 is a criterion of the redistribution of the short and longlived components.

λ_1^{sp} is the mean rate of the spontaneous (stimulated) annihilation; K is the trapping coefficient; $n(\Delta w_L)$ is the bulk spectral density of the stimulating soft photons $(w_L \pm \Delta w_L)$, $\Delta w_L \ll w_0$ is the frequency interval of the laser beam; w_0 is the frequency of the 511-KeV gamma-quanta; $\theta/\Delta\sigma$ depends on the experimental geometry; A is the normalizing integral of the spectral distribution.

Our theoretical model suggests the following experimental results: spatial distribution anisotropy of the annihilation gamma-quanta; change of the intensity of the long and shortlived components of the time dependent annihilation spectrum; decrease of the mean life time of the positron annihilation in the ortho-quasi-positronium state.

The detection and study of the effects can be performed using the experimental setup for measurements of the positron life-time and the energy distribution of the annihilation gamma-quanta.

POSITRON LIFETIMES IN SOLID AND LIQUID ANTHRACENE

P.C. Jain[a], M. Eldrup[b], and J.N. Sherwood[c]

a) Department of Physics and Astrophysics, University of Delhi, Delhi-11007, India
b) Chemistry Department, Risø National Laboratory, DK-4000 Roskilde, Denmark
c) Department of Pure and Applied Chemistry, University of Strathclyde, Glasgow
   G1 1XL, Scotland, UK.

Positron lifetime and Doppler broadening measurements have been carried out on anthracene from room temperature up to a few degrees above the melting point (T_M = 216°C). In crystalline anthracene only one lifetime component could be resolved up to about 5° below the melting point. This component is associated with "free" positrons. Its lifetime increases from 0.320 nsec at 25°C up to 0.350 nsec just below melting. In addition a low intensity ($\lesssim$ 1%) 2-3 nsec component appears within 5°C of the melting point. In the liquid four lifetime components may be resolved of τ_1 = 0.12 ns, τ_2 = 0.415 ns, τ_3 = 1.4 ns, and τ_4 = 3.15 ns with intensities of $I_1 \simeq$ 10%, $I_3 \simeq$ 10%, and $I_4 \simeq$ 30%. Thus, in agreement with an earlier less detailed study[1] we conclude that in crystalline anthracene no Ps is formed (except maybe close to the melting point) while Ps is formed in the liquid. Particularly interesting is the presence of two longlived components in a liquid which suggests two different ortho-Ps states. This was previously found also in liquid SF_6[2]. The Doppler broadening measurements give rise to a slowly increasing S-parameter with temperature in the solid. An abrupt increase in S is observed at the melting point. This is in agreement with the expectation that the formation of para-Ps in the liquid gives rise to a narrow component in the DB spectra. Rapid cooling of the sample from the liquid to room temperature resulted in the appearance of a 5%, 1.35 ns component which remained essentially independent of temperature in the solid. This component may be an effect of lattice defects or possibly of impurities.

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THE AMORPHIZATION OF QUARTZ UNDER NEUTRON IRRADIATION STUDIED BY POSITRON ANNIHILATION.

D.Segers, Mbungu Tsumbu, M.Dorikens, L.Dorikens-Vanpraet
F.Van Brabander and A.Van den Bosch*

 I.N.W., Proeftuinstraat 86, B-9000 Gent, Belgium
*S.C.K.-C.E.N., Boeretang 200, B-2400 Mol, Belgium

        Positron annihilation lifetime spectra and the Dopplerbroadening of the annihilation line were measured for crystalline alpha-quartz, fast neutron irradiated quartz and vitreous silica. In the lifetime spectrum for crystalline quartz no lifetime component longer than 300ps could be distinguished. After neutron irradiation a long lifetime component occurs, which is ascribed to ortho-positronium pick-off. This pick-off lifetime value and its intensity saturate above total fast neutron doses of 8E19 n/cm2, i.e. in the same region of irradiation doses where amorphization of alpha quartz has been seen. The pick-off lifetime in saturation irradiated alpha-quartz is longer than in vitreous silica while its intensity is a factor of five smaller in the irradiated sample than in the vitreous silica. Our data indicate that the physical state obtained in the saturation irradiated material is different from the one in vitreous silica. The lifetime and Doppler-broadening results can be understood on the basis of a spikelike mechanism for the amorphization process. The huge differences in the lifetime spectra are represented in figure 1.
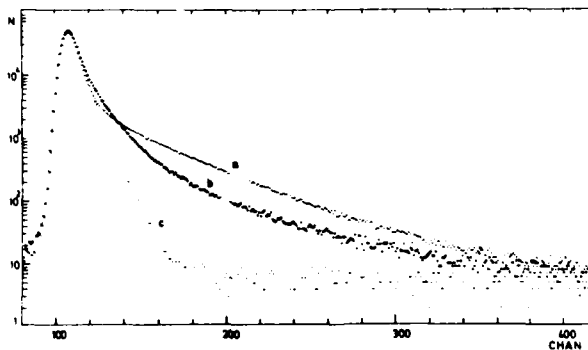
FIGURE 1 :   a) lifetime spectrum for vitreous silica, b) lifetime spectrum for saturation irradiated quartz and c) lifetime spectrum for non-irradiated quartz.

THE SEARCH FOR ANNEALING STAGES OF
VACANCY-TYPE DEFECTS IN GERMANIUM

M. Shimotomai, T. Mihara, K. Oda and M. Doyama

Materials Science, Faculty of Engineering,
The University of Tokyo, Bunkyo-ku, Tokyo, Japan

The knowledge of radiation-induced defects in germanium is still far from maturity largely because of the lack of powerful tools comparable to the ESR and IR techniques for defects in silicon. For example, the annealing stage of divacancies in germanium is of controversy: Some [1] suggests that divacancies are annealed out below room temperature, others [2,3] assign an annealing stage at 400 K to divacancies. We have shown that the sensitivity of positron techniques increases with decreasing measuring temperature owing to the negative temperature dependence of the trapping rate of positrons at defects [4].

In this contribution, we report the Doppler Broadening and positron lifetime measurements of germanium irradiated at liquid nitrogen temperature or at room temperature. The RT-irradiation results suggest that defects introduced by 2 MeV electrons are tri- or tetra-vacancies and the defects do not recover up to 550 K.

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LOW-TEMPERATURE CHARACTERISTICS OF POSITRON
TRAPPING AT DEFECTS IN SEMICONDUCTORS AND GRAPHITE

M. Shimotomai, Y. Ohgino, T. Mihara, K. Inoue and M. Doyama

Materials Science, Faculty of Engineering,
The University of Tokyo, Bunkyo-ku, Tokyo 113, Japan

In solids, positrons dispose of the excess energy relevant to trapping either by electron-hole pair formation or by phonon creation. In semiconductors phonon-mediated trapping is expected to be dominant because of the presence of the forbidden band. Semimetals are interesting in that they represent border-line cases between semiconductors and metals.

We have performed Doppler-broadening and positron-lifetime measurements in the temperature range 4.2-300 K on Si, Ge, GaAs and graphite samples containing defects. The temperature dependence of the trapping rate of positrons are compared with the results of calculation based on the phonon cascade model proposed by Lax.

The trapping rate in Si containing divacancies and one in Ge containing multi-vacancies increase with decreasing temperature in agreement with the prediction of the cascade model. The effect of the charge state of the divacancy in Si on the trapping rate is found. The trapping rate in GaAs irradiated with 2 MeV electrons is weakly dependent on temperature. This could be explained by analogy of multiphonon process of charge carriers in GaAs. Thermal variation of the trapping rate in graphite is small and depends on the nature of defects.

SELF TRAPPING OF POSITRONS IN IONIC CRYSTALS

A. Barry Kunz
Physical Department
Michigan Technological University
Houghton, Michigan 49931

and

James T. Waber
Department of Materials Science and Engineering
Northwestern University
Evanston, Illinois 60201

Our previous calculations of the annihilation of positrons in NaCl type ionic crystals in the bulk and at vacant cation sites, have yielded excellent agreement between theory and experiment for one interpretation of the three lifetimes in NiO. However, the longest component in the lifetime spectra has not accounted for it in our work.

In the present study, local distortion of the charges in the anion coordination shell by the positron indicates that the overlap of the electronic wave functions plays a significant role. There is only very low binding energy when the cation vacancy is monovalent as in AgCl.

On the basis of how electron holes are trapped in Ionic Solids, we have studied positron modelled V_k system and find that the e^+ is bound.

POSITRON ANNIHILATION IN PLASTICALLY DEFORMED SILICON

S. Dannefaer[a], N. Fruensgaard[a], S. Kupca[b], B.G. Hogg[b], D.P. Kerr[b]

a) Institute of Physics, University of Aarhus, DK-8000 Aarhus C, Denmark
b) Department of Physics, University of Winnipeg, Winnipeg, Manitoba, Canada

Positron lifetime and Doppler broadening experiments have been conducted on silicon specimens which were subjected to various degrees of plastic deformation. The deformation temperature was 800°C.

With increasing amount of plastic deformation (from 2,5% to 38%) the trapping rate per unit dislocation concentration decreased from 8×10^{15} sec^{-1} to 4×10^{15} sec^{-1} as measured at room temperature. This is somewhat higher (by a factor of four) than normally calculated for metals.

Two annealing stages were identified by isochronal annealing. One stage was situated at 725-775°C, i.e. below the temperature of deformation, and was characterized by a first order process with an activation energy of 1.4-2.0 eV. The other annealing stage was situated at 825-970°C. Isothermal annealing showed that the activation enthalpy here was 3.5 $\pm$0.3 eV, and is yet another indication for a low value of the self-diffusion enthalpy.

Measurements in the temperature range 15-673°K show that the positron parameters (lifetimes, intensities, and S-parameter) vary strongly with temperature, and that the functional form of this variation is related to the state of annealing of the deformed samples.

It will be argued that in deformed silicon two main types of defects are present. One type consists of isolated vacancy clusters yielding a rather long lifetime of 470 psec. The other type is associated with dislocations and has a trapping cross-section which decreases strongly (as $T^{-1.5}$) at temperatures larger than 120°K. The lifetime of positrons trapped by these defects decreases with temperature and is indicative of a temperautre dependent defect configuration (see figure).

Measuring Temperature ($^{\circ}$K)
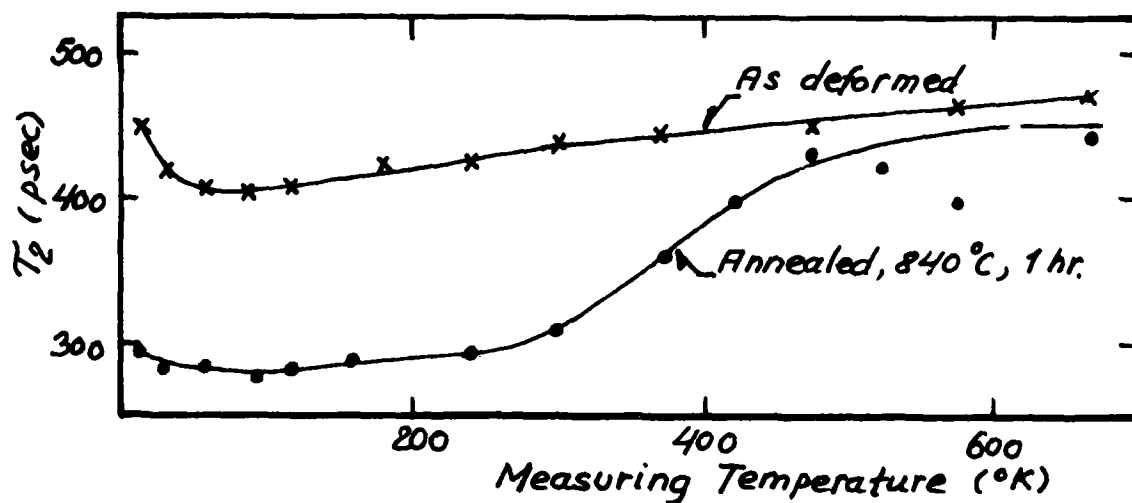
POSITRON LIFETIME INVESTIGATIONS ON HIGH-CRYSTALLINE PTFE IN THE TEMPERATURE REGION BETWEEN -190°C AND 420°C

P. Kindl, H. Sormann, W. Puff

Institut für Kernphysik, Technische Universität Graz
Steyrergasse 4, A-8010 Graz, Austria

The present work reports positron lifetime measurements of the semicrystalline polymer Polytetrafluoroethylene (PTFE) with high degree of crystallinity (>90%) between -190°C and 420°C.

The lifetime spectra were resolved into four components. The obtained lifetimes and intensities are compared with the corresponding data of previous experiments on quenched PTFE with high amorphous content ($\approx$50%)[1,2].

The influence of the crystallinity is obvious if one considers the behaviour of the longest-lived component (τ_4, I_4) which is assigned to the pickoff annihilation of ortho-positronium. At room temperature, the fourth intensity in the high-crystalline material amounts to about 8% - in contrast to 18% in the quenched samples - and changes only slightly up to the melting point (327°C). This is due to the absence of a secondary crystallization, which is just responsible for the significant decrease of I_4 in PTFE with high amorphous content above 100°C. The lifetime τ_4 shows in both cases a similar temperature dependence, whereby however - as to be expected - the values for the high-crystalline material are smaller.

Surprisingly, the third component (τ_3, I_3) has no dependence on the crystallinity (lateral order of the molecular chains). With this fact in mind, and from the marked behaviour of I_3 at the room temperature phase transition and tightly before the melting point, the conclusion can be drawn that this component is most likely sensitive to alterations of the intramolecular structure of the material.

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POSITRON ANNIHILATION STUDIES OF
ZEOLITES ENCAPSULATING HIGH PRESSURE OF KRYPTON

Yasuo Ito, Takemi Takano
Tokai Division, Research Center for Nuclear
Science and Technology, University of Tokyo,
Tokai-mura, Ibaraki-ken, 319-11, Japan

Hironao Kojima
Faculty of Engineering, Yamanashi University,
Takeda, Kofu, Yamanashi-ken, 400, Japan

Shingo Matsuoka, Hirone Nakamura
and Takaaki Tamura
Faculty cf Engineering, University of Tokyo,
Tokai-mura Ibaraki-ken, 319-11, Japan

During our studies of stabilization of krypton gas
in zeolites, which is one of the important subjects in
the waste management in nuclear fuel cycles, we applied
the positron annihilation technique to probe the encap-
sulated krypton state in zeolite.   Although the positron
annihilation technique is still premature to be used for
such an application, some insight into its potential
usefulness and problems have been obtained.

Molecular Sielv-3A which consists of large (α cage)
and small (β cage) cavities was processed with krypton
gas at a high temperature (500-700 C) and high pressure
(500-1000 atm).   Krypton was encapsulated into both
cavities up to 17 wt.%, corresponding to about 250 atm
of Kr in them.   It was also possible to eliminate
selectively the Kr gas in the α cage leaving about 4 wt.%
of Kr only in the β cage.

The result of the positron annihilation measurement
was;

1)   o-Ps intensity becomes larger when MS-3A encapsulates
Kr gas.   This resembles the rise of o-Ps intensity
observed when a small amount of H_2O was absorbed to
zeolites.   This latter result was explained by a
decreased effect of surface active sites due to H_2O
attachment.   Kr is known to be adsorbed to zeolite
only slightly.   It requires further experiment to
examine whether the rise of o-Ps intensity due to
encapsulated Kr is explained in the same way as for
H_2O.   Density effect is an alternative explanation.

2)   The lifetime of o-Ps component was almost the same
for MS-3A and MS-3A containing Kr only in the β
cage.   This suggests that o-Ps prefers α cage
probably because its size is larger.

Further experimental results using other types of
zeolites will also be presented.

A STUDY OF POSITRON ANNIHILATION IN CYCLODEXTRINS

P. K. Tseng, K. S. Chen, and S. Y. Chuang*
Physics Department, National Taiwan University
Taipei, Taiwan, China

*Presently at the Department of Physics, University of
Texas at Arlington, Arlington, Texas 76019

The peak-count of ACAR and Positron lifetime measurements in α- and β-cyclodextrins under various pressure of O_2 and N_2 gases have been investigated. The lifetime spectra can be decomposed into three lifetime components and are similar to those reported previously[1],[2]. In the case of O_2 absorbed samples, the only significant change observed was the intensity I_3 of the long-lived τ_3-component which decreased as the pressure of O_2 was increased. The counting rate of the peak-count experiment was also decreased with the increase of O_2 pressure. This result proves that O_2 molecules absorbed in cyclodextrins inhibit the formation of positronium as proposed by Hadley et al[2]. Both peak-count and lifetime measurements showed little or no changes for the sample under several atmospheres of N_2 gas pressure. This confirms that N_2 molecules do not get into the voids of cyclodextrins to form a clathrate compound.[3]

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DISTRIBUTION OF MOISTURE IN NYLON SPECIMENS USING ENERGY-SELECTED POSITRONS

William H. Holt and Willis Mock, Jr.
Naval Surface Weapons Center, Dahlgren, VA 22488, U.S.A.

Jag J. Singh
NASA Langley Research Center
Hampton, Virginia 23665
U.S.A.

MORE ABOUT POSITRON AND POSITRONIUM LIFETIMES AND INTENSITIES IN 3,3-DIETHYLPENTANE AS A FUNCTION OF TEMPERATURE

S.R. Tuttle, L.M. Diana, P.G. Coleman, S.C. Sharma
S.Y. Chuang, and J.N. McKamy
Center for Positron Studies, Box 19059, UTA Station
The University of Texas at Arlington, Arlington, Texas 76019, U.S.A.

Positron lifetimes in 99% pure 3,3-diethylpentane were measured at twenty-five temperatures from $23.26 \pm 0.21°C$ to $141.74 \pm 0.34°C$. Free positron lifetimes and intensities found at these temperatures were 0.405 ± 0.015 ns and $50.6 \pm 3.3\%$ and 0.453 ± 0.015 ns and $37.7 \pm 1.8\%$ respectively, and orthopositronium lifetimes and intensities were 3.37 ± 0.04 ns and $29.53 \pm 0.24\%$ and 4.36 ± 0.04 ns and $33.16 \pm 0.19\%$ respectively. Orthopositronium annihilation rates and corresponding surface tensions fit the equation $\lambda_3 = (0.073 \pm 0.003) \gamma^{(0.44 \pm 0.01)}$. Results will be discussed in terms of the free volume model.

ON POSITRON STOPPING IN THYLAKOIDS

H. Stachowiak and D. Lehmann[*]
Institute for Low Temperature and Structure Research,
Polish Academy of Sciences,
Pl. Katedralny 1, 50-950 Wrocław, Poland

W. Hendrich
University of Wrocław, Institute of Biochemistry,
ul. Tamka 2, 50-137 Wrocław, Poland

Assuming the present day understanding of the electric potential distribution in leaves in the presence of light[1] it is shown that positrons can be stopped in the membranes separating thylakoids in chloroplasts. Indeed, though the potential differences occuring in thylakoids are not known exactly, the realistic values of the corresponding parameters are sufficient to allow the existence of bound positron states. The positron trapped in such a state could leave the granum only by diffunding along the membrane separating thylakoids. So, the number of annihilations in thylakoids would be much bigger in the presence of light when the membrane can be considered as a defect than in darkness. This could explain the corresponding changes observed in the correlation curves by Dworakowski et al.[2].

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* Present address: Technical University of Dresden, Group for Theoretical Physics, Dresden, GDR.

George Graf and James C. Glass
Departments of Physics and Biochemistry
North Dakota State University
Fargo, North Dakota 58105, U.S.A.

The positron annihilation lifetime technique has been used to investigate conformational changes in proteins by probing the packing density of the molecule. Conformational changes are investigated as a function of temperature, pH and ligand binding. Studies of carbonic anhydrase, ribonuclease and hemoglobin are reviewed, and recent data on ATP binding to (Na^+K^+)ATPase are presented.

POSITRONS IN BIO-MOLECULAR SYSTEMS II

James C. Glass and George Graf
Departments of Physics and Biochemistry
North Dakota State University
Fargo, North Dakota 58105, U.S.A.

The positron annihilation lifetime technique has been used to investigate structural transitions in model membranes by probing the packing density of these systems. Studies of synthetic phospholipid bilayer vesicles are reviewed and recent data presented in an investigation of the anesthetic effects of nitrous-oxide on phospholipid molecules in liposome suspensions. Results suggest a more solid-like nature of the lipid bilayer in the presence of nitrous-oxide.

AUTHOR INDEX