



The International Workshop on Positron Studies and Defects 2017 (PSD-17)

September 3 to September 8, 2017 Dresden, Germany

Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Program

Welcome	p 01
PSD-17 Committees	p 02
General Information	p 05
Presentation Guidelines	p 06
Social Program	p 07
Overview Program	p 08 - 09
Detailed Program	p 11 - 22
Poster Sessions Program	p 23
Abstracts of Oral Presentations	p 25 - 74
Abstracts of Poster	p 75 - 86
Participants List	p 87



MARTIN-LUTHER-UNIVERSITÄT



HALLE-WITTENBERG



Welcome

Dear participants of the Workshop,

It is a great pleasure to welcome you to the International Workshop on Positron Studies of Defects 2017 (PSD-17). The aims of this workshop are to bring together positron scientists who are studying defects in materials for various applications and to provide an international platform to present and discuss recent results and achievements as well as on new experimental and theoretical methods in this field.

This year Dresden hosts the 9th workshop in the series of PSSD/PSD workshops which was established in 1987 in Wernigerode, Germany. The conference site in the following years then moved from Halle / Germany (1994) to Hamilton / Canada (1999), Sendai / Japan (2002), Coeur d' Alene / USA (2004), Prague / Czech Republic (2008), Delft / The Netherlands (2011) to Kyoto / Japan (2014).

We are sure that now the historic environment of Dresden, the regional capital of the Free State of Saxony, offers a perfect place to create a stimulating atmosphere of exciting talks, inspiring discussions, and scientific curiosity by combining the cultural heritage and tradition of the former royal residence for the Electors and Kings of Saxony, who for centuries furnished the city with cultural and artistic splendor with one of the largest agglomerations of academic education and research institutions in Germany. Institutes from the Max Plank Society, the Fraunhofer Society, the Leibniz Association, and the Helmholtz Association are well connected among one other as well as with the academic education institutions lead by the Technical University of Dresden, and of course with the local enterprises of "Silicon Saxony" like Infineon, Globalfoundries (former AMD), ZMDI, and others.

The conference excursion will take us up the Elbe river basin to the picturesque Elbe Sandstone Mountains and onto the Königstein Fortress at the hilltop which offers a splendid view into the valley and which is one of Saxony's foremost tourist attractions. We hope that you have enough time to explore the city of Dresden, its museums, churches, castles, gardens, and other spots by your own as well.

We would like to thank the members of the International Advisory Committee for their guidance and advice. We hope that we have compiled an interesting and stimulating program which shall foster the scientific exchange across the globe and helps to establish new contacts or collaborations.

We also would like to thank the team of Intercom GmbH for professional help in the organization of the conference. Our special thanks go to Ms. Anne Varga, our conference secretary, for her continuous and professional organization during the preparation of the conference, and moreover for her endless patience and commitment.

Last but not least, we would like to thank you all for your contributions and your enthusiasm while presenting your newest results to our community.

We wish you all an exciting and fruitful stay in Dresden!

Andreas Wagner and Reinhard Krause-Rehberg

On behalf of the Organizing Committee of PSD-17

Dresden and Halle, August 2017



PSD-14 Committees

Local Organizing Committee:

- Andreas Wagner (chair)
- Reinhard Krause-Rehberg (co-chair)
- Maciej Oskar Liedke
- Maik Butterling
- Anne Varga (conference secretary)

International Advisory Committee:

- Jakub Cizek (Charles University, Prague, Czech Republic)
- Christoph Hugenschmidt (TU Munich & FRM II, Germany)
- Reinhard Krause-Rehberg (Martin-Luther University Halle, Germany)
- Kelvin G. Lynn (Washington State University, Pullman, USA)
- Peter Mascher (McMaster University, Canada)
- Henk Schut (Delft University, The Netherlands)
- Yasuharu Shirai (Kyoto University, Japan)
- Filip Tuomisto (Aalto University, Helsinki, Finland)

General Information

Conference venue

The conference hall is located at the campus of Helmholtz-Zentrum Dresden-Rossendorf about 15 km from downtown Dresden. Public transportation stops in front of the lecture hall. A free bus transfer is organized from and to the HZDR. It starts every morning at 8:00 in front of the Pullman Hotel (first time on Monday morning) and returns at 18:00.

Registration

The registration starts on Sunday at 16:00 in the Pullman Hotel where we will also have our Get-Together-Party between 18:00 and 20:00. The registration is continued Monday morning at the conference venue. Provided that you did not pay the registration fee yet, please make sure to be on Sunday between 16:00 and 18:00 at the registration desk at Pullman Hotel.

Internet Access

WLAN (WIFI) will be available at the conference hall, poster area, the canteen, and in the guesthouse.

The SSID is: conference
and the password: Yellow46850NorwayMaple

Moreover, your usual login at the EDUROAM network will also work.

Lunches and Coffee breaks

Lunch will be provided in the canteen of the Helmholtz-Zentrum Dresden-Rossendorf.

Monday - Thursday, Sep-04 - Sep-07: from 12:20 - 14:00
Friday, Sep-08: from 12:20 - 13:00

Coffee Service is available in front of the conference hall.

Monday - Friday, Sep-04 - Sep-08: from 10:30 - 11:00
Friday - Tuesday, Sep-04 - Sep-05: from 15:30 - 16:00
Wednesday, Sep-06: from 15:40 - 16:00

Lab Tour

On Wednesday , Sep-06, from 16:00 - 17:30 we will provide a guided Lab Tour through the Positron Facilities of the HZDR. We will start from the conference hall.

Presentation Guidelines

Oral presentations

All presentations will be held in the Conference Hall in the Helmholtz-Zentrum Dresden-Rossendorf (HZDR).

The presentation times are:

- Invited: 30 min (including 5 min discussion)
- Oral: 20 min (including 5 min discussion)

Speakers will not be allowed to exceed their presentation time, so please make sure that you stay within the presentation time limit.

We recommend to operate your presentations from our PC (Office installed).

Poster

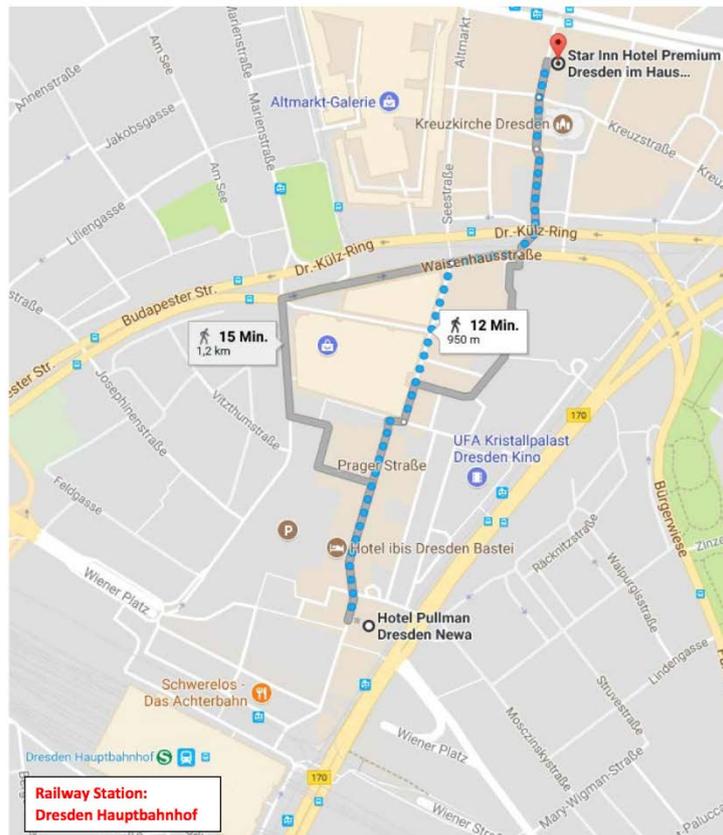
Please prepare your posters in format A0 / portrait and hang them up until Monday lunch break. We have only a small number of posters. Thus, we will have no extra poster session. The posters will be displayed in front of the lecture hall entrance until Wednesday. Please use especially the afternoon coffee break to visit the posters. We would explicitly encourage you to bring recent results on posters with you.

Social Program

Get-Together-Party

Date: Sunday, Sep-03, 18:00 - 20:00

Venue: Pullman Hotel (see Hotel Map)



Walking distances:

Railway Station	to Hotel Pullman – 5 min	to IBIS Hotel – 5 min	to Star Inn Hotel – 16 min
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Star Inn Hotel	To Hotel Pullman – 12 min
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Opening

Date: Monday, Sep-04, 09:00 - 09:30

Venue: Conference hall, HZDR

Conference Excursion

Date: Thursday, Sep-07, 14:00 - 21:30

Venue: We will visit the Fortress Königstein, a hilltop fortress near Dresden. It is one of the largest hilltop fortifications in Europe and sits atop the table hill of the same name.

There we will have our Conference Dinner.

Workshop Program - Overview

Overview Program: Sunday, Sep-03 - Tuesday, Sep-05

		Sunday (Sep-03)	Monday (Sep-04)	Tuesday (Sep-05)
08:00	00	Bus Transfer Hotel → HZDR		
09:00	00		Opening Session	V. Slugen I-05
	10			
	20			
	30		J. Kuriplach I-01	M. Fujinami I-06
	40			
10:00	50			
	00		F.A. Selim I-02	A. Nozaki I-07
	10			
	20		Registration	
	30		Coffee Break	Coffee Break
11:00	40			
	50			
	00		K. Senthilkumar O-01	K. Sugita O-11
	10		B.Y. Wang O-02	B.Y. Wang O-12
	20		L.Y. Dubov O-03	V. Krsjak O-13
12:00	30			
	40		A.M. Ibrahim O-04	M. Butterling O-14
	50			
	00		Lunch	
	10			
13:00	20			
	30			
	40			
	50			
	00			
14:00	00		M.O. Liedke I-03	R. Ferragut I-08
	10			
	20		G. Zagler O-05	I. Prochazka O-15
	30		P. Maheshwari O-06	P.M.G. Nambissan O-16
	40			
15:00	50			
	00		K. Siemek O-07	E. Hecht O-17
	10			
	20		Coffee Break / Poster Session	
	30			
16:00	40			
	50		X.Z. Cao I-04	C. Naidoo I-09
	00	Registration	P. Hruška O-08	N. Sakata I-10
	10			
	20		T. Toyama O-09	
30	M. Liu O-10			
40				
17:00	50			
	00			M. Nippa O-18
	10			
18:00	00	Get Together	Bus Transfer HZDR → Hotel 18:00	
20:00	00			

Session:

Semiconductors	Oxides	Metals	Porous Systems
Alloys	Techniques	Steels	Al Alloys

Workshop Program - Overview

Overview Program: Wednesday, Sep-06 - Friday, Sep-08

		Wednesday (Sep-06)	Thursday (Sep-07)	Friday (Sep-08)	
08:00	00				
09:00	00	J. Čížek I-11	C. Hugenschmidt I-16	G. Schramm Plenary Talk	
	10				
	20				
	30	T.E.M. Staab I-12	M. Dodenhöft I-17		
	40				
50			T.S. Kavetsky O-28		
10:00	00	M. Elsayed I-13	A. Yabucchi B. I-18	S. Aghion O-29	
	10				
	20	Coffee Break			
	30				
	40				
50					
11:00	00	T.E.M. Staab O-19	M. Saro O-25	C. Evans I-19	
	10	G. Klinser O-20	E. Hirschmann O-26		
	20				
	30	X. Zhang O-21	M. Petriska O-27	Arutyunov I-20	
	40				
50					
12:00	00	L. Chiari O-22	Conference Photo	Closing Session	
	10				
	20	Lunch			
	30				
	40				
50					
13:00	00	IAC Meeting			
14:00	00	P.J. Simson I-14	Bus Transfer to Fortress Königstein	Bus Departure 13:00	
	10				
	20				
15:00	30	S. Ishibashi O-23			
	40	A. Yabuuchi O-24			
	50	A. Wagner I-15			
16:00	00	Coffee Break			
	10	Lab Tour			Workshop Dinner
	20				
	30				
	40				
50					
17:00	00	Busses return to Hotels 21:30			
	10				
	20				
18:00	00				
20:00	00				

Session:	Semiconductors	Oxides	Metals	Porous Systems
	Alloys	Techniques	Steels	Al Alloys

Workshop Program - Oral presentations / Details

Sunday, September 3rd

Venue: Pullman City Hotel

16:00 - 20:00	Registration
18:00 - 20:00	Get together

Monday, September 4th

Venue: HZDR lecture hall

08:00	Bus Transfer Hotel → HZDR
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09:00 - 09:30	Opening R. Sauerbrey (Scientific Director of the HZDR) A. Wagner (Head Nuclear Physics Division, Chair of Workshop)
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09:30 - 10:30	General Semiconductors I	Chair: A. Wagner
09:30 - 10:00	J. Kuriplach <i>Invited</i> (Charles University Prague, Czech Republic) <i>“Positronium affinity as a sensitive probe of materials electronic structure”</i>	I-01 p. 25
10:00 - 10:30	F.A. Selim <i>Invited</i> (Bowling Green State University, USA) <i>“Positron Annihilation Measurements of Origin of Novel Electronic Phenomena in Semiconductors and Oxides”</i>	I-02 p. 26

10:30 - 11:00	Registration / Coffee Break
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Workshop Program - Oral presentations / Details

Monday, September 4th (Continued)

Venue: HZDR lecture hall

11:00 - 12:20	Semiconductors II	Chair: P.J. Simpson
11:00 - 11:20	K. Senthilkumar (National Institute of Technology Meghalaya, India)	O-01 p. 27
	<i>“Study on Vacancy Defects in ZnO Nanoparticles by Coincidence Doppler Broadening Spectroscopy”</i>	
11:20 - 11:40	B.Y. Wang (Multi-discipline Research Center Beijing, China)	O-02 p. 28
	<i>“Influence of Cu content on the structure of ZnS:Cu thin films by sulfuration”</i>	
11:40 - 12:00	L.Y. Dubov (National Research Center “Kurchatov Institute” - ITEP, Moscow)	O-03 p. 29
	<i>“Evolution of defect structure in proton irradiated Si during aging studied by PALS and FTIR spectroscopy”</i>	
12:00 - 12:20	A.M. Ibrahim (Martin-Luther-Universität Halle-Wittenberg, Germany)	O-04 p. 30
	<i>“Defect Study in Copper Indium Gallium Selenide (CIGS) by positron annihilation spectroscopy”</i>	

12:20 - 14:00	Lunch
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14:00 - 15:30	Alloys I	Chair: V. Slugen
14:00 - 14:30	M.O. Liedke (Helmholtz-Zentrum Dresden-Rossendorf, Germany)	<i>Invited</i> I-03 p. 31
	<i>“Magnetic phase transitions in ns-laser irradiated FeAl systems: the role of open volume defects”</i>	
14:30 - 14:50	G. Zagler (Technische Universität München, Germany)	O-05 p. 32
	<i>“Vacancy formation in the Heusler system Ni₂ MnAl_{1-x}[Ga[□]]</i>	

Workshop Program - Oral presentations / Details

Monday, September 4th (Continued)

Venue: HZDR lecture hall

Alloys I (Continued)	
14:50 - 15:10	P. Maheshwari O-06 p. 33 (Bhabha Atomic Research Centre Mumbai, India) <i>“Positron annihilation studies on thermally activated Cr precipitation in NiCr binary alloy”</i>
15:10 - 15:30	K. Siemek O-07 p. 34 (Joint Institute for Nuclear Research Dubna, Russian Federation) <i>“Positron Annihilation and Complementary Studies of Dental Alloys Exposed to Sandblasting”</i>
15:30 - 16:00 Coffee Break / Poster Session	
16:00 - 17:30	Metals I Ag Alloys I Chair: J. Čížek
16:00 - 16:30	X.Z. Cao I-04 p. 35 <i>Invited</i> (Institute of High Energy Physics Beijing, China) <i>“Effect of helium irradiation dose on He_nV_m clusters evolution in nickel studied by positron annihilation spectroscopy”</i>
16:30 - 16:50	P. Hruška O-08 p. 36 (Charles University Prague, Czech Republic) <i>“Slow positron annihilation studies of Pd-Mg multilayers”</i>
16:50 - 17:10	T. Toyama O-09 p. 37 (Tohoku University Ibaraki, Japan) <i>“Deuterium trapping at vacancy clusters in neutron-irradiated tungsten studied by positron annihilation spectroscopy”</i>
17:10 - 17:30	M. Liu O-10 p. 38 <i>“Artificial ageing and subsequent secondary natural ageing in an Al-0.4Mg-0.4Si alloy”</i>
18:00	Bus Transfer HZDR → Hotels

Workshop Program - Oral presentations / Details

Tuesday, September 5th

Venue: HZDR lecture hall

08:00	Bus Transfer Hotel → HZDR
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09:00 - 10:30	Steels I Metals II	Chair: P.M.G. Nambissan
09:00 - 09:30	V. Slugen (University of Technology in Bratislava, Slovak Republic)	<i>Invited</i> I-05 p. 39
	<i>“Influence of the initial microstructure on vacancy clustering in neutron irradiated Fe-Cr alloys and steels.”</i>	
09:30 - 10:00	M. Fujinami (Chiba University, Japan)	<i>Invited</i> I-06 p. 40
	<i>“The Critical Defects Induced in bcc- and fcc-iron on Hydrogen Embrittlement by Positron Annihilation Spectroscopy”</i>	
10:00 - 10:30	A. Nozaki (Chiba University, Japan)	<i>Invited</i> I-07 p. 41
	<i>“Hydrogen-induced defects in α-iron by positron annihilation lifetime spectroscopy”</i>	

10:30 - 11:00	Coffee Break
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11:00 - 12:20	Steels II	Chair: M. Fujinami
11:00 - 11:20	K. Sugita (Osaka University, Japan)	O-11 p. 42
	<i>“Hydrogen detection in steels using positron lifetime spectroscopy”</i>	
11:20 - 11:40	B.Y. Wang (Institute of High Energy Physics Beijing, China)	O-12 p. 43
	<i>“Study of microdefects in ion irradiated FeCrNi alloy by positron annihilation”</i>	

Tuesday, September 5th (Continued)

Venue: HZDR lecture hall

Steels II (Continued)	
11:40 - 12:00	V. Krsjak O-13 p. 44 (Slovak University of Technology, Slovakia) <i>“Positron study of helium effects in FeCr alloys irradiated in different radiation environments”</i>
12:00 - 12:20	M. Butterling O-14 p. 45 (Helmholtz-Zentrum Dresden-Rossendorf, Germany) <i>“Characterization of the irradiation-induced microstructure in Fe-based model alloys and reactor pressure vessel steels by means of Gamma-induced positron annihilation spectroscopy (GiPS)”</i>
12:20 - 14:00	Lunch
Oxides I Chair: T.E.M. Staab	
14:00 - 14:30	R. Ferragut <i>Invited</i> I-08 p. 46 (Politecnico di Milano, Italy) <i>“Study of stable subsurface oxygen in copper electrodes during electrochemical CO₂ reduction”</i>
14:30 - 14:50	I. Prochazka O-15 p. 47 (Charles University Prague, Czech Republic) <i>“Defects and porosity in zirconia-based nanomaterials: a study by slow-positron beam technique”</i>
14:50 - 15:10	P.M.G. Nambissan O-16 p. 48 (Saha Institute of Nuclear Physics, Kolkata, India) <i>“Positron Annihilation Studies of a Transition Metal Oxide Nanocomposite $xV_2O_5 - (1-x) (0.05MoO_3 - 0.95ZnO)$”</i>
15:10 - 15:30	E. Hecht O-17 p. 49 (Technische Universität München, Germany) <i>“Defects in oxide single crystals and oxide heterostructures studied by Doppler broadening spectroscopy”</i>

Workshop Program - Oral presentations / Details

Tuesday, September 5th (Continued)

Venue: HZDR lecture hall

15:30 - 16:00	Coffee Break / Poster Session		
16:00 - 17:20	Techniques I Porous Systems I	Chair: C. Evans	
16:00 - 16:30	C. Naidoo	<i>Invited</i>	I-09 p. 50
	(iThemba LABS, South Africa)		
	<i>“Improvements in the Production of ²²Na Positron Sources at iThemba LABS”</i>		
16:30 - 17:00	N. Sakata	<i>Invited</i>	I-10 p. 51
	(Chiba University, Japan)		
	<i>“Positron annihilation lifetime spectroscopy in various kinds of zeolites”</i>		
17:00 - 17:20	M. Nippa		O-18 p. 52
	(Chiba University, Japan)		
	<i>“Change in Free Volume in Strained Rubber with Carbon Black Filler by in situ Positron Annihilation Lifetime Spectroscopy”</i>		
18:00	Bus Transfer HZDR → Hotels		

Workshop Program - Oral presentations / Details

Wednesday, September 6th

Venue: HZDR lecture hall

08:00	Bus Transfer Hotel → HZDR
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09:00 - 10:30	Al alloys II	Chair: R. Ferragut
09:00 - 09:30	J. Čížek (Charles University Prague, Czech Republic)	I-11 p. 53
	<i>“Natural ageing and early precipitation stages in Al-Si-Mg alloys studied by positron annihilation spectroscopy”</i>	
09:30 - 10:00	T.E.M. Staab (University Würzburg, Germany)	I-12 p. 54
	<i>“A detailed atomic investigation of the clustering process on a Friction-Stir-Welding simulated Al-Cu-Li(-Mg) alloy (AA2198) by Positron Annihilation Spectroscopy, SAXS and DSC”</i>	
10:00 - 10:30	M. Elsayed (University Halle-Wittenberg, Germany)	I-13 p. 55
	<i>“Influence of highly diluted alloying elements on the formation of vacancies in aluminum”</i>	

10:30 - 11:00	Coffee Break
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11:00 - 12:20	Al alloys III	Chair: M. Butterling
11:00 - 11:20	T.E.M. Staab (University Würzburg, Germany)	O-19 p. 56
	<i>“Vacancy Binding to Solute Atoms and Stability of Cu-Precipitation in AlCu Alloys”</i>	
11:20 - 11:40	G. Klinser (Graz University of Technology, Austria)	O-20 p. 57
	<i>“Ageing Processes in the Aluminium Alloy AW6060 (Al-Mg-Si) Studied by Positron Annihilation and High-Precision Dilatometry”</i>	

Wednesday, September 6th (Continued)

Venue: HZDR lecture hall

Al alloys III (Continued)	
11:40 - 12:00	X. Zhang O-21 p. 58 (Technische Universität Berlin, Germany) <i>“Effect of Sn on the ageing kinetics of Al-Mg-Si alloys”</i>
12:00 - 12:20	L. Chiari O-22 p. 59 (Chiba University, Japan) <i>“Interaction between dislocations and impurities in strained aluminium by positron annihilation spectroscopy”</i>

12:20 - 14:00	Lunch
13:30 - 14:00	Meeting of the International Advisory Committee

14:00 - 15:40	Semiconductors III Techniques II	Chair: R. Krause-Rehberg
14:00 - 14:30	P.J. Simpson <i>Invited</i> (The University of Western Ontario, Canada) <i>“Silicon Quantum Dots in Silicon Nitride Formed by Solid State Precipitation”</i>	I-14 p. 60
14:30 - 14:50	S. Ishibashi (Research Center for Computational Design of Advanced Functional Materials, AIST, Tsukuba, Japan) <i>“Computational study of correlation between local structures and positron annihilation parameters for cation vacancies in nitride semiconductor alloys”</i>	O-23 p. 61
14:50 - 15:10	A. Yabuuchi (Research Reactor Institute, Kyoto University, Japan) <i>“Study of Ion-Beam-Synthesized β-FeSi₂ Films Probed by a Slow Positron Beam”</i>	O-24 p. 62

Workshop Program - Oral presentations / Details

Wednesday, September 6th (Continued)

Venue: HZDR lecture hall

Semiconductors III Techniques II (Continued)	
15:10 - 15:40	A. Wagner <i>Invited</i> I-15 p. 63
	(Helmholtz-Zentrum Dresden-Rossendorf, Germany)
	<i>"Positron Annihilation Studies using a Superconducting Electron LINAC"</i>

15:40 - 16:00	Coffee Break
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16:00 - 17:30	Lab Tour
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18:00	Bus Transfer HZDR → Hotels
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Thursday, September 7th

Venue: HZDR lecture hall

08:00	Bus Transfer Hotel → HZDR
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Techniques III		Chair: F. Selim
09:00 - 09:30	C. Hugenschmidt <i>Invited</i> I-16 p. 64	
	(Technische Universität München)	
	<i>"Defect Imaging Using the Positron-Microbeam of the CDB Spectrometer at NEPOMUC"</i>	
09:30 - 10:00	M. Dodenhöft <i>Invited</i> I-17 p. 65	
	(Technische Universität München)	
	<i>"Novel Reflection High-Energy Positron Diffractometer at NEPOMUC"</i>	

Workshop Program - Oral presentations / Details

Thursday, September 7th (Continued)

Venue: HZDR lecture hall

Techniques III (Continued)	
10:00 - 10:30	A. Yabuuchi <i>Invited</i> I-18 p. 66 (Research Reactor Institute, Kyoto University, Japan) <i>“The estimation of positron production and heat generation in KUR beam line by PHITS”</i>

10:30 - 11:00	Coffee Break
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Techniques IV		Chair: C. Hugenschmidt
11:00 - 11:20	M. Saro O-25 p. 67 (Slovak University of Technology, Slovakia) <i>“Application of LYSO scintillators in positron annihilation spectroscopy”</i>	
11:20 - 11:40	E. Hirschmann O-26 p. 68 (Helmholtz-Zentrum Dresden-Rossendorf, Germany / Martin Luther University Halle-Wittenberg, Germany) <i>“Digital data acquisition for positron lifetime measurements”</i>	
11:40 - 12:00	M. Petriska O-27 p. 69 (Slovak University of Technology, Slovakia) <i>“Positron lifetime triple coincidence filtering”</i>	

12:00 - 12:20	Conference Photo
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12:20 - 14:00	Lunch
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14:00 - 21:30	Excursion to Fortress Königstein and Conference Dinner
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21:30	Bus Transfer HZDR → Hotels
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Workshop Program - Oral presentations / Details

Friday, September 8th

Venue: HZDR lecture hall

08:00	Bus Transfer Hotel → HZDR
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09:00 - 10:30	Plenary Talk Porous Systems II	Chair: J. Kuriplach
09:00 - 09:50	G. Schramm (KU Leuven, Belgium)	<i>Plenary Talk</i> PT p. 70
	<i>“Positron Emission Tomography - an introduction and overview about current developments”</i>	
09:50 - 10:10	T.S. Kavetsky (Drohobych Ivan Franko State Pedagogical University, Ukraine / The John Paul II Catholic University of Lublin, Poland)	O-28 p. 71
	<i>“Slow positron beam spectroscopy study of PMMA nanocomposite films with ion-synthesized silver nanoparticles”</i>	
10:10 - 10:30	S. Aghion (Politecnico di Milano, Italy)	O-29 p. 72
	<i>“Positron Annihilation Spectroscopy for the study of polymer brushes”</i>	

10:30 - 11:00	Coffee Break
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11:00 - 12:00	Porous Systems III Semiconductors IV	Chair: T.S. Kavetsky
11:00 - 11:30	C. Evans (Politecnico di Milano, Italy)	<i>Invited</i> I-20 p. 73
	<i>“Development of self-standing mesoporous thin films for positronium formation in transmission”</i>	
11:30 - 12:00	N. Arutyunov (Martin Luther University Halle-Wittenberg, Germany/ Institute of Electronics, Uzbekistan/ Ioffe Physico-Technical Institute St. Petersburg, Russia)	<i>Invited</i> I-18 p. 74
	<i>“Configurations of Point Defects in Float-Zone n –Type Silicon Irradiated By 0.9-MeV Electrons and 15-MeV Protons”</i>	

Workshop Program - Oral presentations / Details

Friday, September 8th (Continued)

Venue: HZDR lecture hall

12:00 - 12:20	Closing Session
12:20 - 13:00	Lunch
13:00	Bus Transfer HZDR → Hotels

Poster	First Author	Poster Title	Page
P1	J. Kuriplach <i>Charles University Prague, Czech Republic</i>	Defects in High Entropy HfNbTaTiZr Alloys Studied with Positrons	p. 76
P2	F. Lukac <i>Institute of Plasma Physics/ Charles University Prague, Czech Republic</i>	Defects in high entropy alloy HfNbTaTiZr prepared by spark plasma sintering	p. 77
P3	O. Melikhova <i>Charles University Prague, Czech Republic</i>	Hydrogen-induced defects in Ti and their thermal stability	p. 78
P4	V.S.M. Pereira <i>Delft University of Technology, Netherlands</i>	Doppler Broadening analysis of defect evolution in Eurofer97 and ODS Eurofer97 after He-implantation and annealing treatments	p. 79
P5	G.M.Tanzi <i>Università degli Studi di Milano, Italy</i>	A two-particle model for Positronium confined in sub-nanometric cavities	p. 80
P6	M. Elsayed <i>University Halle, Germany/ Minia University, Egypt</i>	Identification of defects in high-entropy alloys by positron annihilation spectroscopy	p. 81
P7	C. Naidoo <i>iThemba LABS, South Africa</i>	Improvements in the Production of ^{22}Na Positron Sources at iThemba LABS	p. 82
P8	R.S. Laptev <i>National Research Tomsk Polytechnic University, Russia</i>	Positron Spectroscopy of Intermetallic Hydrogen Storage Alloys Synthesis Based on Ti-Cr with C14 and C36 Laves Phases	p. 83
P9	A.M. Lider <i>National Research Tomsk Polytechnic University, Russia</i>	Positron Spectroscopy of Defect Structure Additively Manufactured Titanium Ti-6Al-4V	p. 84
P10	R. Krause-Rehberg <i>University Halle, Germany</i>	Improvement of depth resolution of VEPAS by a simultaneous sputtering technique	p. 85

Positronium affinity as a sensitive probe of materials electronic structure

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The positronium affinity (A_{Ps}) [1], called also the positronium formation potential [2], is defined in terms of the electron (ϕ_-) and positron (ϕ_+) work functions and the Ps ground state binding energy ($E_{\text{Ps}} \cong 6.803$ eV) as

$$A_{\text{Ps}} = \phi_- + \phi_+ - E_{\text{Ps}} .$$

If this affinity is negative, Ps atoms spontaneously leave the surface of a material bombarded with slow positrons. Even if the Ps affinity is defined through surface-related properties, it is a bulk characteristic since the sum $\phi_- + \phi_+$ can be expressed via the sum of electron and positron chemical potentials, which are accessible from density functional theory (DFT) calculations.

The maximum kinetic energy of emitted Ps atoms $E_{\text{K}} = -A_{\text{Ps}}$. In a recent experiment [1], the (110) surface of copper has been studied, and E_{K} has been determined using precise Ps time of flight measurements. Comparing experimental results with the corresponding accurate DFT calculations based on several exchange-correlation (XC) functionals and the recent parameter-free model for gradient-corrected electron-positron correlations [3] results in finding the proper XC functional for Cu with a precision of order 10 meV.

In the present contribution, we continue with copper calculations and test other XC functionals including the recently introduced meta-generalized-gradient approximation [4]. On this basis, we predict A_{Ps} for selected elemental materials and discuss whether Ps emission could be observed. Positron defect studies may also benefit from Ps affinity examination since it can reveal adequate XC functionals to be employed in computations of defect characteristics.

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Positron Annihilation Measurements of Origin of Novel Electronic Phenomena in Semiconductors and Oxides

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Positron Annihilation Spectroscopy (PAS) is known as an effective tool to probe vacancy defects in solids. However when combined with other techniques, PAS becomes really a powerful tool for revealing and explaining many interesting electronic phenomena. Defects play the main role in determining the electrical, optical and magnetic properties of semiconductors and oxides. We combined PAS with transport and magnetic measurements as well as with infrared, optical and luminescence spectroscopies to study the electronic properties of ZnO bulk and thin films. The measurements showed that defects induce ferromagnetism in transition metal doped ZnO films and they are solely responsible for providing the magnetic moments and coupling them. The study also revealed an unusual magnetic hysteresis and a novel magnetic phenomenon in ZnO thin films co-doped with cobalt and aluminum. Examples of our recent PAS measurements of origin of intriguing electronic phenomena in other oxides will be also discussed.

Study on Vacancy Defects in ZnO Nanoparticles by Coincidence Doppler Broadening Spectroscopy

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Positron annihilation technique is a well known non-destructive and highly sensitive probe to study defects in semiconductors [1,2]. One can study the electron density distribution, electron momentum distribution and nature of defects by employing the positron annihilation techniques. In the present work the coincidence Doppler broadening (CDB) spectroscopic technique was applied to study the electron momentum distribution of positronium in ZnO nanoparticles (NPs). For this study, two set of nominally undoped ZnO NPs were prepared by dc arc plasma technique with different oxygen rich conditions such as 760 Torr and 150 Torr pressure with all other parameters were kept constant [3]. Hard pallets have been prepared by using these NPs with high pressure of ~220 MPa. About 10 μ Ci ²²Na source encapsulated in a thin 1.5 micron nickel foil is used as a positron source. The positron source has been sandwiched between two identical pallets of ZnO powder. For the CDB study two high resolution HPGe detectors (PGC 1216sp of DSG) has been used and the data were recorded in a dual ADC based multi-parameter system. The CDB spectra of ZnO sample has been analyzed by constructing the area normalized ratio curve with respect to the CDB spectra of a 99.9999 % pure Al single crystal as shown in Figure 1.

Figure 2 shows the momentum range $p_L \sim 12 \times 10^{-3} m_0c$ to $19 \times 10^{-3} m_0c$ for the 760T sample with respect to 150T sample suggest less annihilation of positrons with the core electrons of Zn in 760T sample. This ratio curve clearly indicates more number of Zn vacancies (V_{Zn}) in 760T sample than the 150T sample. The energy of electron corresponding to this momentum range is 37 eV to 92 eV. This can be identified as the of 3p electron of Zn (88 eV). Thus the present CDB analysis clearly suggests more V_{Zn} related defect complex in 760T sample compared to 150T sample. These results were agreed with recently studied Raman spectra [3].

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The authors are pleased to acknowledge D. Sanyal, Variable Energy Cyclotron Centre, Kolkata for providing the positron annihilation studies.

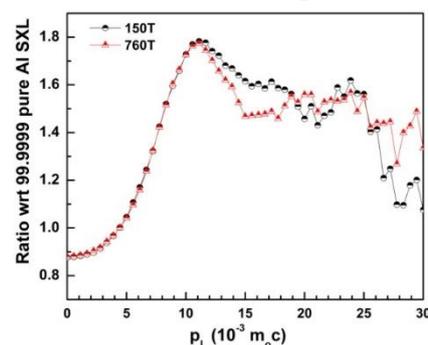


Figure 1. Ratio curve of CDB spectrum for 750T & 150T with respect to 99.9999% pure Al single crystal.

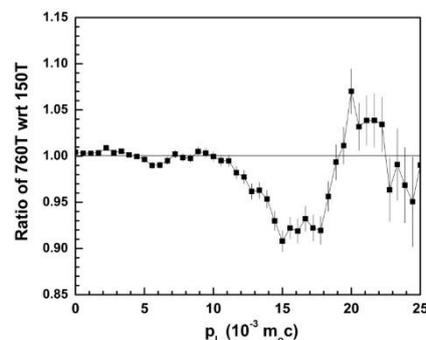


Figure 2. Ratio curve constructed from the CDB spectrum for 750T with respect to 150T ZnO.

Influence of Cu content on the structure of ZnS:Cu thin films by sulfuration

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ZnS:Cu thin films were prepared at 440°C by sulfuring Zn:Cu thin films which grown by magnetron sputtering with zinc target covering different area of copper foil. The structures of prepared samples were investigated by the techniques such as XRD, AFM, SEM and slow positron annihilation spectroscopy technology. In the meantime, the influencing mechanism of pre-treatment and content of copper on the structure of ZnS:Cu thin films was discussed. As the area of copper increases, the morphology ZnS:Cu thin films becomes more uniform and dense. Meanwhile, the grains of ZnS:Cu keep small size and the crystal structure of samples is mainly blende. Along with the increase of the content of copper film, S parameters of the film reduced by degrees. Owing to lower mobility of copper atoms that inhibit the mass aggregation of zinc, the aggregation in Zn:Cu films gradually disappear.

After sulfuring thin film with higher content of copper, the surface pore become less and defect concentration decreases. It indicates that content of copper has a significant impact on ZnS:Cu films by sulfidation. As a result of annealing on prefabricated Zn:Cu films that has the similar effect like higher content of copper, prefabricated Zn:Cu films tend to the improvement of surface morphology. However, according to the S parameter of the ZnS:Cu, the content of Cu play a dominant role in the quality improvement of ZnS:Cu. Although the annealing on Zn:Cu prefabricated films can improve the quality of samples, the similar effect of Cu element on the structure of samples is more apparent. In the pretreatment of the samples, with the increase of the content of copper, S - W curve tends to be linear. It shows that the type of the defects in thin film tend to be single.

Evolution of defect structure in proton irradiated Si during aging studied by PALS and FTIR spectroscopy

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In this work we study annealing of radiation defects in 2 years-aged proton-irradiated silicon. Initial defect structure was formed using irradiation of Cz-Si wafers (400 μm) by protons (21.6 MeV) with the fluence of 1.2×10^{16} proton/cm² [1]. Initial PALS spectra of the irradiated wafers were practically identical, showing that the defect structure in those wafers is the same. Afterwards the wafers have been aged at room temperature and subjected to isochronous step-wise annealing from 20 to 750 °C. Aging time was 1 month for the first sample of the irradiated wafers, 14 months for the second sample, and 22 months for the third sample. The samples have been examined by PALS and FTIR spectroscopy at room temperature after each step of annealing.

At annealing temperatures below 250 °C the positron lifetime in defects τ_d is about 280-290 ps due to annihilation of positrons in divacancies (V_2) of disordered regions (DR). For temperatures less than 150 °C only weak annealing of V_2 is observed, while decrease of the trapping rate κ occurs much faster (Fig.1). For the longer aged silicon wafers (samples 2 & 3) we notice the local increasing of trapping rate in DR (at 60 °C and 120 °C respectively).

When V_2 become mobile they interact with interstitial oxygen (O_i) and with A-centers (VO) thus forming V_2O and V_3O . These complexes are the main trapping centers for positrons up to 400°C. Concentration of V_2O and V_3O in sample 3 appeared to be essentially lower than in the first two samples that indicate a decrease in the concentration of vacancy-type defects during the aging process. When VO, V_2O and V_3O are completely annealed at 400 °C and VO_2 complexes are formed we observed unexpected behavior of the e^+ trapping rate in the sample 3. Although FTIR spectra indicate that concentration of VO_2 after annealing at 500°C does not change, the e^+ trapping rate increases significantly.

The raise of the lifetime associated with the formation of multi-vacancy clusters in the sample 3 begins much later. This also confirms that the total number of vacancy-type defects in the long aged irradiated Si decreases.

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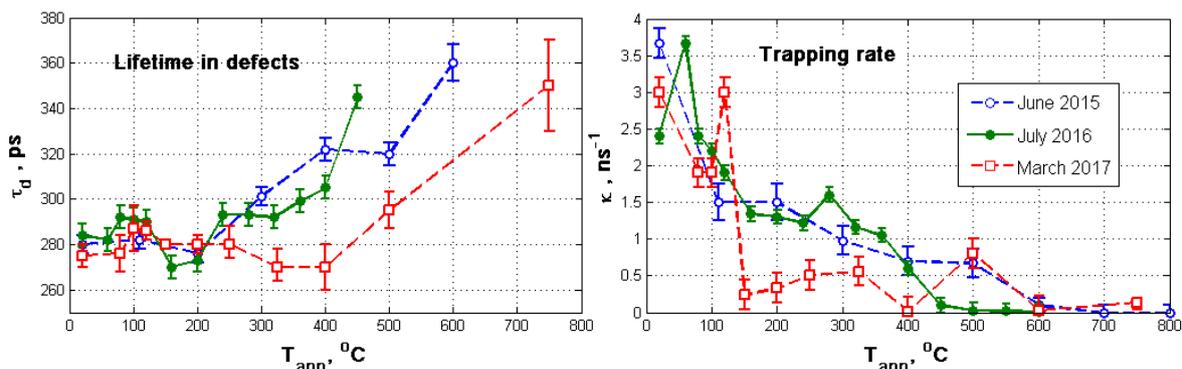


Fig. 1. Annealing of the samples with different time of aging.

Defect Study in Copper Indium Gallium Selenide (CIGS) by positron annihilation spectroscopy

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CIGSe based solar cells are currently very good candidates for a new generation thin films photovoltaic. CIGSe has recently achieved a record efficiency of 22 % [1], however, the theoretically predicted value is 31 % [2]. The analysis of structure property relations is a crucial task for further development of these devices due to the chemical complication of the compound. Therefore deeper understanding of their physical properties, which strongly depend on the defect properties, will allow improving the solar cell efficiency. In this work three series of samples have been investigated by the positron annihilation spectroscopy.

Cu (In_xGa_{1-x}) Se₂ films, grown under various Se fluxes exposed to illumination from a halogen lamp, CIGSe with different Cu contents (with and without Na diffusion) and CIGSe with various Ga concentration have been investigated with positron annihilation spectroscopy. The line-shape parameter (S) of the positron annihilation spectra was used to characterize the defects in the CIGS films. The metastability phenomenon was not confirmed in the first series as Lany and Zunger expected [3]. On the other hand When Cu ratio was decreased, the S parameter increased, also by permitting Na from the SLG substrate to diffuse into the film, S parameter decreased. For the third series, it was noticed that, there are optimum values of Ga concentration which give low S parameter.

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Magnetic phase transitions in ns-laser irradiated FeAl systems: the role of open volume defects

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Fe₆₀Al₄₀ alloys exhibit disorder dependent magnetic phase transitions (MPT), e.g., a ferromagnetic disordered A2-phase turns into a paramagnetic ordered B2-phase [1]. The ordered B2-phase, formed due to annealing up to 500°C in vacuum can be reversed to the disordered A2-phase via ion-irradiation [2]. It has been shown that the physical origin of MPT is related to the so-called anti-site disorder (ASD), i.e., variations in the number of Fe-Fe nearest neighbors due to disordering of the system [3]. However, variations of the lattice parameter, secondary phases, and changes in the concentration and size of open volume defects may play an important role as well. Here, an excimer UV ns-laser has been utilized to induced defects and examine the role of ASD and defects onto magnetic properties of Fe₆₀Al₄₀. Samples of 40 nm thick Fe₆₀Al₄₀ films with different initial order levels were exposed to a range of laser fluences: (i) Ne⁺ irradiated fully-disordered (A2- Fe₆₀Al₄₀), and (ii) vacuum annealed ordered alloys (B2- Fe₆₀Al₄₀) and (iii) as-grown semi-disordered (A2/B2- Fe₆₀Al₆₀). It is seen that for laser pulses of fluences below 100 mJ·cm⁻² cause subtle changes to the magnetization depending on the Fe₆₀Al₄₀ initial state, whereas for fluences above 150 mJ·cm⁻², strong increase in ferromagnetism is observed for all Fe₆₀Al₄₀ initial states. The laser irradiated samples were probed with the Positron Annihilation Spectroscopy (PAS) to analyze for the existence of vacancies and/or phase separation. Although the low fluence region shows nearly no variation in vacancy defect concentration, a slight increase in the number of Al atoms around defect sites is found. For the high fluence regime, it is seen that a large variation in vacancy defects occurs, followed by pronounced phase separation. Structural analysis of the phase separated films shows strong migration of Al atoms leaving behind Fe-enriched regions, consistent with the PAS spectra.

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Vacancy formation in the Heusler system $\text{Ni}_2\text{MnAl}_{1-x}\text{Ga}_x$ G. Zagler¹, M. Leitner^{1,2}, P. Neibecker^{1,2}, C. Hugenschmidt^{1,2}¹Technische Universität München, Physics Department, 85748 Garching, Germany²Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II), 85748 Garching, Germany
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Heusler alloys are ternary intermetallic compounds with the sum formula X_2YZ , displaying extraordinary phenomena such as the ferromagnetic shape memory effect (FSME). The FSME is caused by field-induced magneto-structural reorientation where the structural and magnetic degrees of freedom are coupled. While the prototypical FSM-alloy Ni_2MnGa of L2_1 crystal structure displays a large strain of up to 6%, the closely related Ni_2MnAl -system, given that it is L2_1 ordered, is thought to display the same effect, but lacks the necessary L2_1 crystal structure. It was shown that excess vacancies can speed up the ordering process in the slow-ordering Ni_2MnAl -system [1]. To gain insight into the vacancy formation processes and to compare the vacancy formation energies, Doppler Broadening Spectroscopy (DBS) with in-situ heating was conducted at the NEPOMUC beamline of FRM II for Ni_2MnGa , Ni_2MnAl and the intermediate $\text{Ni}_2\text{MnAl}_{0.5}\text{Ga}_{0.5}$ composition. As can be seen in figure 1, $\text{Ni}_2\text{MnAl}_{0.5}\text{Ga}_{0.5}$ shows a temperature dependent behaviour of the S -parameter which increases linearly due to the lattice expansion until positrons are increasingly trapped in the emerging vacancies. Eventually all positrons are trapped, resulting in saturation trapping. Temperature dependent DBS with variable implementation depth was performed to determine the vacancy concentration and the vacancy formation energy. In addition Coincident DBS at high temperatures allowed us to investigate the types of defects.

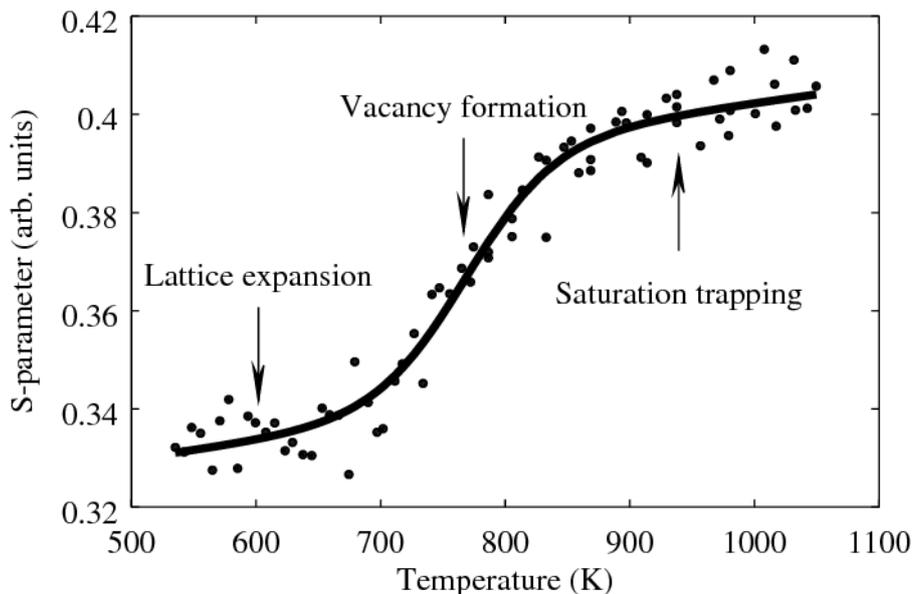
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Figure 1: Temperature dependent S -parameter of $\text{Ni}_2\text{MnAl}_{0.5}\text{Ga}_{0.5}$ due to an increasing vacancy concentration at higher temperatures, measured with 28 keV positrons.

Positron annihilation studies on thermally activated Cr precipitation in NiCr binary alloy

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NiCr alloys are a class of materials with excellent corrosion and radiation resistance as well as mechanical properties. The solubility of Cr in Ni declines sharply with decreasing temperature resulting in phase separation of a supersaturated γ -matrix upon ageing at a given temperatures. The precipitation of α -Cr, which is a Cr-rich phase with bcc structure, affects the mechanical properties and the corrosion resistance of the alloy. In the present work, the kinetics and mechanism of precipitation (α -Cr) with ageing at different temperatures (650 and 800°C) has been studied using Positron annihilation lifetime and coincidence Doppler broadening (CDB) spectroscopy. The γ -phase of the alloy is obtained by quenching the solid solution of the alloy in water from 1200°C. The as-quenched alloy was aged up to 96 hrs at 650 and 800°C, as the case may be. Although the positron affinity of Cr (-2.62 eV) is higher than Ni (-4.46 eV), the defects formed at the interface of precipitate and the matrix acts as trapping site leading to detection of Cr precipitates sensitively.

Two positron lifetime components corresponding to the annihilation in the γ -matrix (τ_1 , I_1) and open volumes (τ_2 , I_2) present at the interface of the precipitates are obtained. Ageing (650 and 800°C) results in increasing contribution from the open volume defects at the interfaces indicating the nucleation as well as growth of precipitates as a function of ageing time. The evolution of local environment (measured using CDB) and the variation of the size of open volume defects have been correlated to the growth behaviour of the precipitates in terms of coherency at the interface. Both the hardness test and positron annihilation results showed that kinetics of precipitation is slower at lower temperature (ca. 650 °C). The result will be discussed.

**Positron Annihilation and Complementary Studies of Dental Alloys
Exposed to Sandblasting**

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Defect studies of subsurface zone in dental alloys POLYCAST, MAGNUM AN, I-MG, I-GW exposed to sandblasting were performed using positron annihilation spectroscopy techniques. Samples were treated at two different pressures of the air stream 1 and 4 bar. Conventional experiments based on positrons emitted directly from the radioactive source allowed us to detect vacancies on the dislocation edges in all samples, however, the total depths of subsurface zones depended on the pressure, i.e., for I-MG 22 μm for pressure of 1 bar and about 43 μm for 4 bar. The complementary methods such as SEM and AFM revealed also dependencies between the pressure of the air stream and roughness of the surface. The slow positron beam and RBS measurements showed oxide layers after annealing.

Effect of helium irradiation dose on He_nV_m clusters evolution in nickel studied by positron annihilation spectroscopy

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Austenitic stainless steels have good corrosion resistance, resistant to high and low temperature, which have been applied in various industries widely. The most important application is to be the candidate structural material for fission reactors. It is well known that the helium were easily generated by (n, α) nuclear reaction. High dose of helium and formation of helium bubbles in the structural materials could enhance void swelling, surface blistering and degrade mechanical properties. The component of austenitic stainless steels was complicated, in order to investigate effect of helium irradiation dose in structural material. Therefore, nickel, as a typical face centered cubic material, was used and could avoid interference of component of materials. In the present study, nickel was cut to the size of $10 \times 10 \times 1 \text{ mm}^3$. Mechanical polishing and electrochemical polishing were used to make specimen having a fine mirror-like surface. And then, the specimens were annealed at 1223 K for 2 h with a high vacuum ($\sim 10^{-5}$ Pa), followed by air cooling. Helium irradiation was carried out using 50 keV helium ions at the room temperature, and the dose was $1 \times 10^{17} \text{ He}^+/\text{m}^2$, $1 \times 10^{18} \text{ He}^+/\text{m}^2$ and $1 \times 10^{19} \text{ He}^+/\text{m}^2$, respectively.

After helium irradiation, many vacancies were introduced in the specimen, and helium-vacancy (He_nV_m) clusters were formed due to the combination between vacancies and helium atoms. Positron annihilation Doppler Broadening spectroscopy (DBS) was used to characterize the irradiation-induced defects evolution because the positrons were easily trapped by irradiation-induced defects and annihilated with electron around irradiation-induced defects.

The mono-energetic positrons of DBS were implanted into the specimens with the energy changed from 0.1 to 20 keV. The S-E plot shows that the S parameter was increased after helium implantation, which indicate that vacancy type defects generated. The S-W plot shows that size of He_nV_m increased with helium irradiation dose.

Acknowledgements

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Slow positron annihilation studies of Pd-Mg multilayers

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Palladium is well known for its excellent hydrogen absorption kinetics. The gravimetric hydrogen absorption capacity of Pd is however only 0.93 wt. %. Magnesium exhibits a high hydrogen absorption capacity up to 7.6 wt. %, however the hydrogen absorption kinetics is slow. The aim of this work was to create thin Pd-Mg multilayered films combining positive hydrogen absorption properties of both elements.

Pd-Mg multilayers were deposited by RF magnetron sputtering on fused silica substrates coated with 100 nm thick Pd wetting layer. The multilayers consist of alternating Pd and Mg layers (3, 12 and 60) of the same thickness. Three types of Pd-Mg multilayers were compared: (i) as deposited samples, (ii) hydrogen gas loaded samples at room temperature and H₂ pressure of 4000 Pa for 2 h, (iii) samples annealed up to 450°C under Ar atmosphere.

Defect structure of Pd-Mg multilayers was characterized using variable energy positron annihilation spectroscopy. Doppler broadening of the annihilation photopeak was analyzed using the S and W line-shape parameters and the measured S(E) curves were fitted using the VEPFIT code. The development of the structure during the annealing of the films was monitored by in-situ X-ray diffraction. Atomic force microscopy was employed for the study of the surface morphology. All films were characterized by nanocrystalline structure with a high density of grain boundaries with open-volume defects capable of positron trapping. The density of grain boundaries is determined by the mean grain size which increases with increasing thickness of a single phase layer. Hydrogen loading led to buckling of the film and introduced additional defects into the film. Annealing of the multilayers leads to diffusion of Mg atoms into the Pd layers and precipitates of Mg-Pd phase are formed.

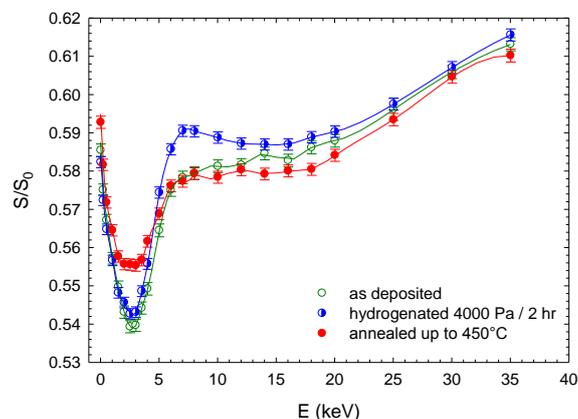


Fig. 1: Dependence of the S parameter on the positron energy for 12-layered Pd-Mg multilayer.

Deuterium trapping at vacancy clusters in neutron-irradiated tungsten studied by positron annihilation spectroscopy

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Deuterium trapping at irradiation-induced defects in tungsten, a candidate material for plasma facing components in fusion reactors, was revealed by positron annihilation spectroscopy. Pure tungsten was neutron-irradiated (at 573 K to a dose of ~ 0.3 dpa), followed by post-irradiation annealing at 573 K for 100 hours. Annealing was performed in a vacuum or in deuterium gas at ~ 0.1 MPa. Positron lifetime for the latter was shorter than that for the former, suggesting deuterium trapping at vacancy clusters. To reveal this, coincidence Doppler broadening measurements were performed. Figure 1 shows the correlation between the low momentum component fraction (LCF) and high momentum component fraction (HCF) of all samples. The dashed straight line connects correlation points between the Un-irradiated and the As-irradiated samples, which are representative of positron annihilation in tungsten bulk and vacancy clusters in tungsten, respectively. For the four samples, the correlation points are located on the dashed line, indicating positron annihilation only for tungsten electrons. Conversely, the correlation point for the sample annealed in deuterium gas after irradiation is located below the dashed line. Such low HCF must be due to positron annihilation with deuterium electrons, because deuterium possesses no core electrons. Thus, deuterium trapping at irradiation-induced vacancy-clusters was observed, which is expected to cause significant increase in deuterium retention in irradiated-tungsten.

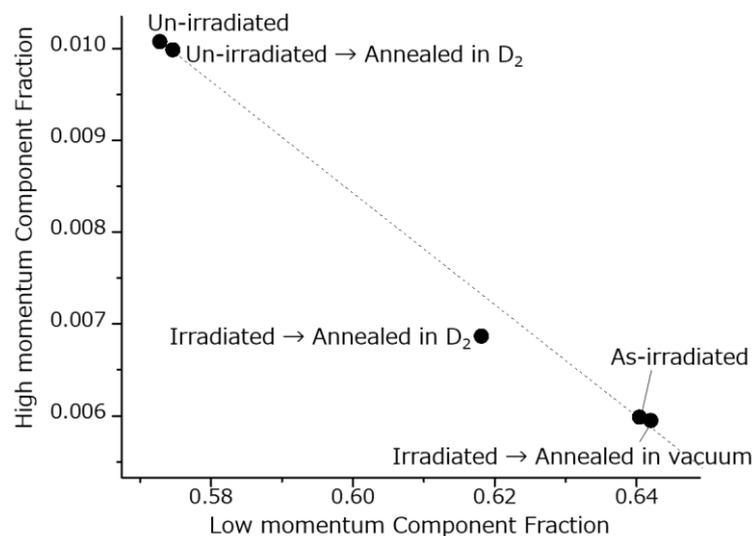


Fig. 1: Correlation of low momentum component fraction (LCF) and high momentum component fraction (HCF) of coincidence Doppler broadening measurements.

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Artificial ageing and subsequent secondary natural ageing in an Al-0.4Mg-0.4Si alloy

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Positron annihilation lifetime spectroscopy (PALS) was applied to investigate the phenomenon of secondary natural ageing (SNA) in an Al-0.4Mg-0.4Si (wt.%) alloy after ageing treatments at 180 °C for various times. The notable change in positron lifetime during the early stage of SNA indicates that shortly after solution treatment and quenching (~2 min), the loss of quenched-in vacancies and the formation of solute clusters/GP zones/precipitates are markedly accelerated by ageing the alloy in an oil bath even for just 2 seconds. A qualitatively similar effect was observed by replacing oil with liquid BiSn, but in this case, vacancies disappear even more rapidly, arising from the much higher heat conductivity of BiSn than oil. We also found that further SNA was the strongest when the alloy was aged for 5 min. The positron lifetime effect was discussed as a function of ageing time and a model was suggested to explain the interplay of vacancies and solute atoms.

Influence of the initial microstructure on vacancy clustering in neutron irradiated Fe-Cr alloys and steels.

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The influence of the initial microstructure (ferrite vs. ferrite/martensite) on evolution of vacancy type defects in various iron-chromium model alloys and high chromium ferritic/martensitic steels have been studied using coincidence Doppler broadening spectroscopy. Besides the role of the alloying elements on response of the material to irradiation, the initial microstructure of Fe-Cr alloys and steels present another factor that affects the open volume defects evolution and mechanical properties degradation after neutron irradiation.

Specimens were neutron irradiated to 0.11 dpa at two different temperatures, 290°C and 450°C. It has been found that at irradiation temperature $T_{\text{irr}} = 290^\circ\text{C}$, the initial microstructure (ferrite vs. ferrite/martensite), in particular dissolved carbon distribution within the matrix is one of the key factor that affect response of the materials to neutron irradiation, especially in terms of vacancy cluster formation in Fe-Cr alloys and steels. Presence of dissolved carbon within the matrix leads to formation of stable and immobile carbon-vacancy complexes which act as traps for irradiation induced vacancies and therefore, leading to increased formation of vacancy clusters. Internal friction (IF) and magnetic after-effect (MAE) studies revealed that, as manifestation of the different initial microstructure, C atoms were distributed differently within the matrix of the pure ferritic vs. ferritic/martensitic alloys. Namely, while in the ferritic alloys most of the C atoms were distributed uniformly within the matrix and ready to interact with irradiation defects creating strong and stable CVa complexes, in ferritic/martensitic alloys the matrix was virtually free of C, where most of it had segregated at the martensite lath boundaries and grain boundaries. Therefore all alloys and steels with pure ferritic microstructure exhibit higher level of open volume defects compared to specimen with ferritic/martensitic microstructure.

Correlation between initial microstructure and evolution of open volume defects has also been supported by results of $T_{\text{irr}} = 450^\circ\text{C}$ measurements where level of open volume defects in all alloys and steels decreased to the level of non-irradiated state due to dissociation of CVa complexes that occurs, as reported by various authors, at 400-430°C.

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The Critical Defects Induced in bcc- and fcc-iron on Hydrogen Embrittlement by Positron Annihilation Spectroscopy

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It is well known that hydrogen decreases the formation energy of vacancies in metals, resulting in hydrogen embrittlement (HE), but the crucial defect species have never been clarified yet. Positron annihilation lifetime spectroscopy (PALS) is one of the most powerful methods to directly detect open-volume type defects and enables us to gather information on their size, chemical state and amount. The aim of this work is to clarify the crucial defects related to HE in pure α -iron and austenitic stainless steel by PALS.

Pure α -iron (bcc) specimens were deformed at two different strain rates of 2.2×10^{-5} /s and 3.3×10^{-4} /s under a hydrogen environment. The slower the strain rate, the greater is the hydrogen susceptibility. Hydrogen can be easily released from the specimen even at RT and the induced defects may be annealed at RT, so the specimens were quenched at 80 K just after deformation. PALS spectra were measured at different temperatures from 170 K to 520 K. It was found that vacancy clusters with 15 vacancies could be formed in both of the specimens. However, in the specimens deformed at the slowest strain rate the positron lifetime due to vacancy clusters increased from 230 ps to 500 ps as the measurement temperature was raised. These results could be explained by the formation of vacancy-hydrogen complexes, which were considered the dominant defects in HE.

The two types of austenitic stainless steels, SUS 304 and SUS 316L, were pre-charged with hydrogen and subjected to tensile straining. The SUS 304 alloy showed HE, whereas the SUS 316L alloy showed low hydrogen susceptibility. The vacancy clusters could be induced in both of the samples, indicating that they were not crucial in the HE process. By comparing the defect behavior in detail using the PALS method, we can clarify the vacancy-hydrogen complexes which are related to HE in fcc iron.

Hydrogen-induced defects in α -iron by positron annihilation lifetime spectroscopy

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Hydrogen embrittlement (HE) is one of the most serious issues in establishing safe designs in hydrogen energy systems. One of the mechanisms of HE is the enhancement of instability during plastic deformation by strain-induced vacancies. In particular, plastic deformation leads to the formation of dislocations and vacancies and hydrogen reduces the vacancy formation energy and enhances their formation. Hydrogen-induced defects agglomerate and form vacancy clusters, resulting in enhanced instability during plastic deformation. It was found in the previous studies that the formation of the vacancy clusters was promoted in α -iron with bcc crystal structure deformed in a hydrogen environment. It is well known that HE strongly depends on the strain rate. The slower the strain rate, the higher is the HE susceptibility, meaning that hydrogen diffusion and interaction with defects are important in HE. In this study, our aim is to clarify the crucial defects in HE by positron annihilation lifetime spectroscopy (PALS) with a comparison of the slow- and fast-strained iron samples.

Pure (4N) α -iron samples were hydrogen charged while being deformed at two different strain rates of 2.2×10^{-5} /s and 3.3×10^{-4} /s. Hydrogen charging was conducted by cathodic electrolysis at a current density of 50 A/cm² in an aqueous solution of H₂SO₄ of pH 2.5 to which 0.09 wt% NH₄SCN was added. We assume that the critical defects in HE are unstable at room temperature without tensile stress and in the lack of hydrogen. Therefore, both samples were strained up to 16 % and released, followed by aging for 1 hour and quenching at 77 K in order to freeze the induced defects. PALS measurements were carried out between 170 K and 520 K. PALS spectra were fitted with three lifetime components (bulk, dislocations, vacancy clusters).

HE was induced in the slow-strained sample, while the fast-strained sample did not show HE. However, vacancy clusters were detected in both samples, so that the vacancy clusters themselves were not directly responsible for HE. In the slow-strained sample, the lifetime due to vacancy clusters gradually became longer between 250 and 420 K and remained constant from 420 to 520 K, indicating that mobile defects were induced around 250 K. The defects which are mobile around 250 K are monovacancies. However, monovacancies are unstable at RT and they cannot form in the normal tensile test. It was, therefore, concluded that vacancy-hydrogen (VH) complexes are locally formed in HE. After hydrogen is released, the resultant monovacancies agglomerate to form vacancy clusters above 250 K. In the fast-strained sample, the lifetime due to vacancy clusters became longer than that in the slow-strained sample and increased between 300 and 315 K, meaning that there are no mobile defects below 300 K. It was, therefore, concluded that monovacancies do not exist and smaller vacancy clusters are uniformly distributed in the sample. This indicates that VH complexes are not induced in fast-strained pure iron.

In summary, we have investigated the defects induced by plastic deformation in H-charged pure iron and the defect behavior dependence on the strain rate in order to elucidate the crucial defects in HE. From the PALS results, it can be concluded that VH complexes are the crucial defects in HE in α -iron.

Hydrogen detection in steels using positron lifetime spectroscopy

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Even minute amounts of hydrogen in metals have been known to cause hydrogen embrittlement failures in various metals especially high-strength steels. Hydrogen intruded into metals is reported to be trapped by defects, however, it remains unclear how trapped hydrogen plays a critical role in embrittlement failures. For deep understanding of the phenomena developing in-situ techniques for detecting ppm levels of hydrogen and analyzing trap state is of crucial importance.

As with the case of hydrogen, positrons in metals are expected to be trapped by open volume defects i.e., vacancies, voids, dislocations etc. So positron annihilation characteristics (lifetime and Doppler broadening) can be affected by the presence or absence of trapped hydrogen. In this research, positron lifetime spectroscopy was applied to hydrogen-charged steels in order to examine the feasibility of positron annihilation method for detecting ppm levels of hydrogen.

The steels high strength bolt steels with and without vanadium addition were austenitized at 880 / 920 °C and after quenching they were tempered at 600 °C. The steel plates with thickness of 1mm were hydrogen charged by soaking for 48 h at 50 °C in a 20 wt% ammonium thiocyanate solution. The samples maintained for 0-96 h at 25 °C after hydrogen charging were then subjected to thermal desorption spectroscopy (TDS) analysis and positron lifetime spectroscopy. TDS results suggests that the diffusible hydrogen contents were increased by vanadium addition.

Mean positron lifetime of a vanadium-added steel was significantly decreased by hydrogen charging, and then increased gradually accompanied with decreasing of hydrogen contents, and finally became equivalent to a noncharged sample. TDS results demonstrates that the changes in mean positron lifetime correlated with hydrogen contents in a hydrogen-charged vanadium-added steel. Two-component analyses of positron lifetime spectra imply that the positron lifetime of defects is decreased by hydrogen trapping. These results supports that positron annihilation method is a promising nondestructive technique to for detecting and analyzing ppm levels of hydrogen in metals.

Acknowledgements

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Study of microdefects in ion irradiated FeCrNi alloy by positron annihilation

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Austenitic stainless steels are widely used as structural materials in nuclear reactor systems. Neutron irradiation damage, including the formation and evolution of microdefects, are important issues, which related to the degradation of mechanical properties. In present study, ion irradiation were performed to simulate the irradiation damage process. Iron ions and hydrogen ions were implanted into the FeCrNi alloys, respectively. The implantation fluence and irradiation temperature varied during irradiation process. Doppler Broadening based on slow positron beam was used to characterize irradiation induced vacancy type defects.

The S parameters were sensitive to irradiation fluence during heavy ion bombarded. It means that large amount of vacancy type defects formed even at low damage dose, which were defined as damage incubation period. However, the S parameters showed saturated to the variation of damage dose up to 0.05 dpa. The results of TEM showed the formation and growing process of dislocation loops. The results also indicates that hydrogen-vacancy complexes might be formed during hydrogen injection with low irradiation temperature. The irradiation induced vacancies and hydrogen-vacancy complex would be unstable during higher temperature irradiation, and the recovery process of vacancy type defects might proceeded, simultaneously. Isochronal annealing would performed on the as-irradiated specimens to study the evolution and recovery of irradiation induced microdefects.

Acknowledgements

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Positron study of helium effects in FeCr alloys irradiated in different radiation environments

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Fe-12 wt.% Cr model alloy was implanted by 250keV He²⁺ ions to three different fluencies (3×10^{17} , 9×10^{17} and 1.5×10^{18} cm⁻²) at T < 100°C. In a depth profile manner, the implantation peak (Fig.1) profile was investigated using variable energy slow positrons, with the primary focus on the region 100-230nm. The obtained data were compared to Optifer IX samples irradiated in STIP 2 target [1] of Swiss Spallation Neutron Source (SINQ).

The irradiation conditions produced by implantation of helium ions provide an extremely harsh environment, even when compared to spallation targets. While the displacement damage (dose) in the studied helium-implanted samples is comparable to a two-years campaign in the spallation target, dpa rate and helium production rate are increased by orders of magnitude in the He implantation experiments. The concentration of helium is comparable for low-dpa samples, but in the high-dpa implantation sample, it goes well above the spallation conditions.

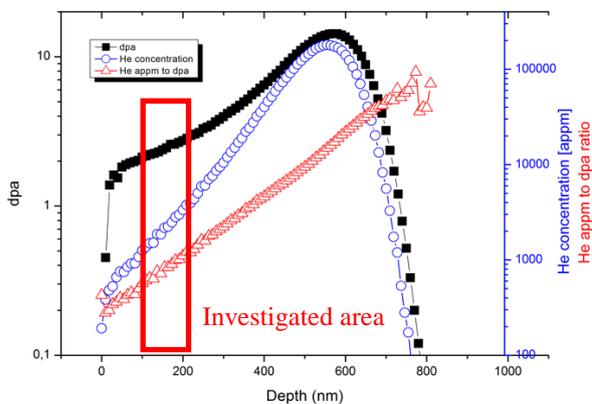


Fig. 1. Displacement damage peak and He profile as simulated by SRIM code.

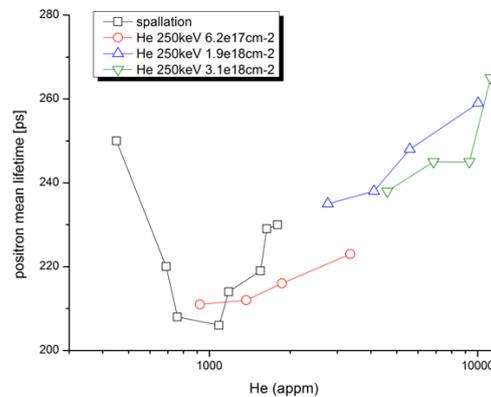


Fig. 2. Average positron lifetime as a function of helium concentration in spallation and He-implanted samples.

The evolution of positron mean lifetime with He appm (Fig.2.) indicate the role of accumulated helium on the formation of complex vacancy-type defect clusters. It also suggests that accelerated displacement damage rate of ion implantations does not produce substantially different defects and at fluence $< 10^{18}$ cm⁻² the values of τ_{av} are very similar to irradiation in spallation environment.

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Characterization of the irradiation-induced microstructure in Fe-based model alloys and reactor pressure vessel steels by means of Gamma-induced positron annihilation spectroscopy (GiPS)

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Components of future fission reactors of the fourth generation and fusion devices will be exposed to higher neutron fluences than the reactor pressure vessel (RPV) and internals of currently operating nuclear power plants. This poses challenges for the selection and qualification of damage tolerant structural materials. Ferritic/martensitic Cr steels are one of the promising candidates because of their favorable resistance against irradiation swelling. As compared to currently used RPV steels, additional effects such as the formation of α' particles, G-like phases or He bubbles are currently in the focus [1]. One particular topic of interest for RPV steels is the occurrence of so-called late-blooming phases [2-4], which can form after long irradiation times and lead to considerable material ageing effects [4]. These phases can occur if factors of certain material composition and irradiation conditions are combined: Low Cu-content, moderate to high Mn- and Ni- content, comparatively low irradiation temperature, high neutron fluence and low neutron flux.

To get information about the irradiation-induced vacancy-type defects in very small clusters (≤ 0.5 nm), positron annihilation spectroscopy plays an important role, because it is the only method that can resolve these defects.

However, neutron exposure of steel leads to the formation of the ^{60}Co isotope which is registered in the positron lifetime spectrum as a prompt curve (two simultaneous gammas). Thus, to obtain a reasonable quality of spectra, a triple coincidence is necessary which can elongate the time for a single spectrum to several days. The GiPS (Gamma-induced positron annihilation spectroscopy) spectrometer avoids this disadvantage, because the start of the lifetime measurement is not registered from a gamma quantum, but originates from the ELBE machine pulse. Thus, only a slight increase of the measurement time is necessary to avoid the overload of the detectors [5]. Another advantage of the GiPS spectrometer compared to conventional setups is the fact that GiPS provides the defect information over the whole sample volume, while isotope sources, like ^{22}Na will have a limited information depth of a few tens of microns. Thus, surface degradation due to sample treatment, corrosion and preferential surface effects will not be important for the GiPS setup.

In the first part of the presentation, we focus on the flux effect of RPV steels where vacancies and vacancy clusters play a key role [6,7]. The second issue is focused on ferritic/martensitic Cr-steels in order to investigate systematically the effect of alloying elements on microstructure evolution under increased irradiation.

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Study of stable subsurface oxygen in copper electrodes during electrochemical CO₂ reduction

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Electrodes formed with nanoparticles of oxide-derived copper (OD-Cu) exhibit higher activity than pristine copper during the electrochemical carbon dioxide reduction reaction (CO₂RR) and, more importantly, possess higher selectivity towards ethylene, which is a valuable product for the chemical industry [1]. The presence of residual subsurface oxygen in OD-Cu has been proposed to be responsible for such improvements, although its stability under the reductive CO₂RR conditions remains unclear.

This work sheds light on the nature and stability of oxygen within the nanoparticles subsurface using positron annihilation spectroscopy (PAS) and *quasi in situ* electron energy-loss spectroscopy (EELS) in a transmission electron microscope (TEM). The oxidized and reduced thin films were characterized by means of a positron slow beam. PAS measurements of S and W parameters and positronium formation yield as a function of positron implantation energy were obtained. In order to identify the chemical environment of defects in the reduced sample, Coincidence Doppler Broadening for a selected positron implantation energy was also used. The resulting spectra show contributions of Cu, Cu₂O and CuO in the reduced sample [2-3].

Our spectroscopic results show that oxygen is primarily concentrated in an amorphous 1-2 nm thick layer within the Cu subsurface. Besides, oxygen is associated with a high density of defects in the OD-Cu structure. We propose that both low-coordination of the amorphous OD-Cu surface and the presence of subsurface oxygen that withdraws charge from the copper sp- and d-bands might selectively enhance the binding energy of CO.

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Defects and porosity in zirconia-based nanomaterials: a study by slow-positron beam technique

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A variety of advantageous thermal, electrical and mechanical properties of zirconium di-oxide (ZrO_2 , zirconia) make zirconia-based materials widely used in many industrial areas, in particular, in ceramic industry and other high-temperature applications. Doping of the ZrO_2 host lattice by proper metal cations is a prerequisite of stabilisation of the high-temperature cubic and tetragonal phases down to room temperature as well as improvement of other functional properties. The use of nanopowders as initial substances in manufacturing ZrO_2 -based nanoceramics by sintering leads to well-homogenised materials of a low porosity. Due to an appreciable volume fraction of grain boundaries (GBs), pores and nanometer-sized open-volume defects associated to GBs become significant in nanopowders. Obviously, positron as well as positronium (Ps) atom becomes efficient probes of microstructure evolution during production of ZrO_2 -based functional nanomaterials by sintering.

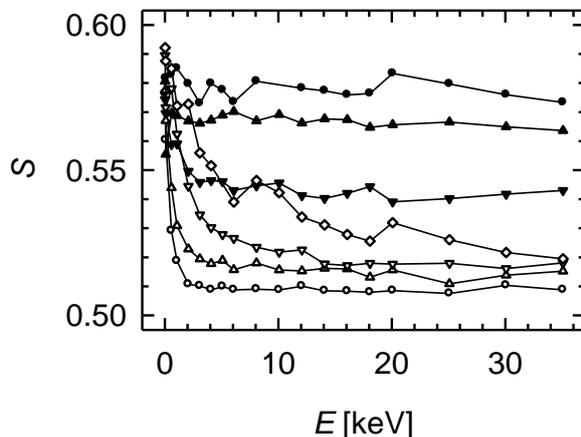


Figure. S -parameters measured for ZrO_2 materials doped with 10 mol.% MgO (triangles), 12 mol.% CeO_2 (circles) and 4 mol.% MgO (diamonds). Full symbols – compacted nanopowders, empty symbols – sintered ceramics.

were fitted to the measured $S(E)$, $W(E)$ curves. The DB experiments were supplemented with the conventional positron lifetime, X-ray diffraction (XRD) and mass-density (MD) measurements. Nature and depth distributions of open-volume defects will be discussed on the basis of the slow-positron beam results correlated with the data on positron lifetimes, XRD and MD.

In the present contribution, investigation of several zirconia-based nanopowders as well as ceramics, obtained by sintering these nanopowders, will be reported. Nanopowders under study were doped with metal cations of various valency (Mg^{2+} , Y^{3+} , Cr^{3+} , Ce^{4+}) and differed also in thermal treatment. Doppler broadening (DB) measurements using slow-positron beam were conducted in the positron energy E ranging from 0.03 eV to 35 keV and the ordinary S and W shape parameters as well as the relative 3γ fractions were evaluated as functions of E . In Figure, an example of measured $S(E)$ curves is given illustrating the sintering induced disappearance of open volume defects and para-Ps formation as well as grain growth could be observed. The VEPFIT models

Positron Annihilation Studies of a Transition Metal Oxide Nanocomposite $x\text{V}_2\text{O}_5 - (1-x)(0.05\text{MoO}_3 - 0.95\text{ZnO})$

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Metal oxide nanocomposite formation and subsequent evolution of nanocrystallites are promising areas of research where positron annihilation spectroscopy has got unique importance in getting information on the vacancy type defects at the cationic sites [1]. In this work, a nanocomposite of the nomenclature $x\text{V}_2\text{O}_5 - (1-x)(0.05\text{MoO}_3 - 0.95\text{ZnO})$ is synthesized through melt-quenching for x ranging from 0 to 0.9 in intervals of 0.1 or 0.2. After the initial characterization with X-ray diffraction, positron lifetime and coincidence Doppler broadening measurements are done in all the samples. XRD spectra indicated the formation of unique nanocrystallites at lower values of x while large scale amorphousness of the composite system was observed for $x = 0.5$ and above.

Positron lifetime spectra yielded three components in each, the third component varying from 0.7 to 4.8 ns being indicative of the presence of ortho-Ps atoms within the free volume defects (Fig. 1). The variation of this lifetime (τ_3) served certain indications to the processes taking place at the different stages of incorporation of V_2O_5 that serves both as a catalyst as well as an active reagent in the formation of newer nanocrystallites. The initial fall and rise of τ_3 is reproduced in repeated measurements and confirmed the presence of interfacial defects around these nanocrystallites. The subsequent fall of τ_3 and increase of I_3 are indicative of the increasing degree of amorphousness and shifts of the sites of ortho-Ps formation from the interfaces to the porous defects.

The steady increase of the defect-specific positron lifetime τ_2 and the intensity I_2 suggests new positron trapping sites being formed (Fig. 1). These nanocrystallite phases have been identified from the XRD results and, from their known crystalline structure, the oxygen electron density parameters directly affecting the lifetimes of positrons trapped within the cationic vacancies are calculated. The observed variation of τ_2 is found consistent and the increased I_2 indicated the availability of such trapping centres in increasing number within the nanocomposites when the concentration of the catalyst V_2O_5 is increased. The CDBS results showed a rise and fall of the heights of the $2p$ electron annihilation peak (at $p_L = 9.8 \times 10^{-3} m_0c$) indicating the dominance of the processes of nanocrystallite formation and amorphousness at the respective stages.

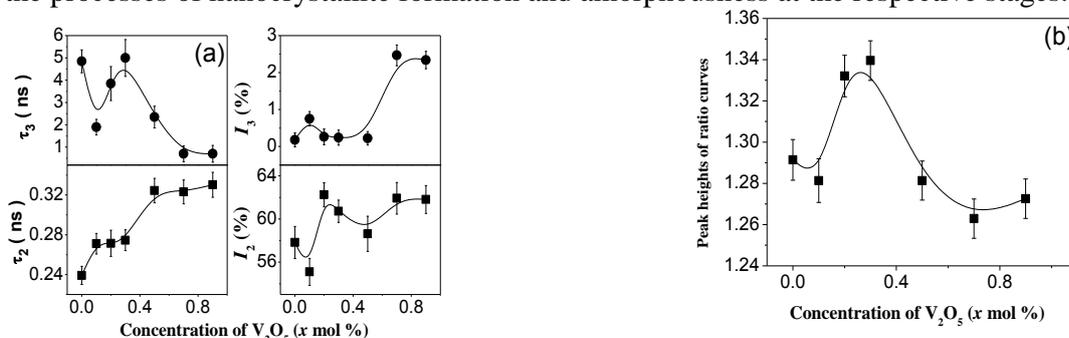


Fig. 1: (a) Positron lifetimes and intensities and (b) the $2p$ electron (O_2^{2-}) annihilation peak heights of the different samples (with different input concentrations of V_2O_5).

Defects in oxide single crystals and oxide heterostructures studied by Doppler broadening spectroscopy

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There is a considerable interest in novel complex oxides and especially heterostructures which exhibit extraordinary properties. In particular the electronic structure at interfaces can be tuned to act as insulators, conductors or even superconductors. Within this study, oxide single crystals as well as various samples of $\text{LaNiO}_3/\text{LaAlO}_3$ (LNO/LAO) heterostructures are examined by a combination of positron beam experiments and ab-initio calculations. High quality LAO/LNO heterostructures with varying layer thickness have been grown by pulsed laser deposition (PLD) and molecular beam epitaxy (MBE). The defects in the various samples have been studied by (coincident) Doppler broadening spectroscopy ((C)DBS). Depth resolved DBS was performed to obtain the S parameter and positron diffusion length of the different layers (Fig. 1).

The experimental found positron diffusion length are used to estimate the relative defect concentration for different growth methods and changing layer thicknesses. CDBS has been carried out to investigate the chemical surrounding of open volume defects. In addition, a novel data analysis software has been developed and tested against the recent software and, for additional verification, against simulations runs with ABINIT. As oxide heterostructures are challenging to simulate additional measurements have been made for comparison on oxide single crystals serving as model systems (for recent ABINIT calculations on oxides see [1]). As a next step it is envisaged to simulate positron annihilation in complex oxides such as LAO and LNO and eventually in the according heterostructures. Our findings are compared to complementary results on similar samples obtained by AFD and XRD [2].

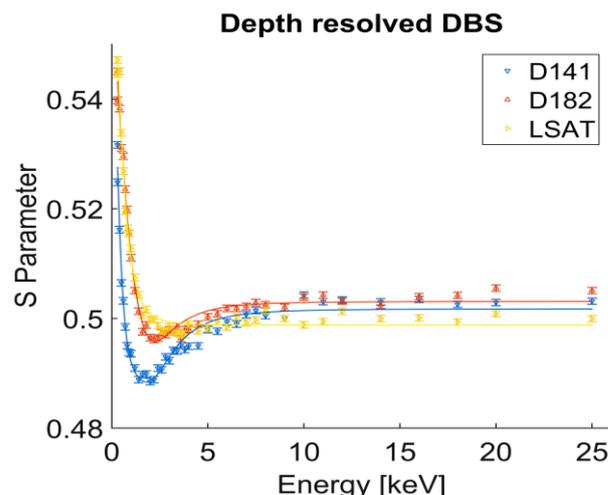


Figure 1: Depth resolved DBS on MBE grown samples with $20 \times [2 \times 2]$ (D141) and $8 \times [4 \times 4]$ (D182) LNO/LAO layers and the substrate LSAT. The positron diffusion length for D141 and D182 was found to be length of 1 nm and 4 nm, respectively.

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

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

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

Positron annihilation lifetime spectroscopy in various kinds of zeolites

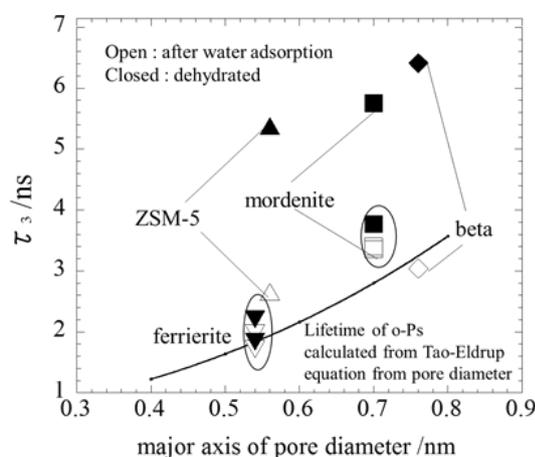
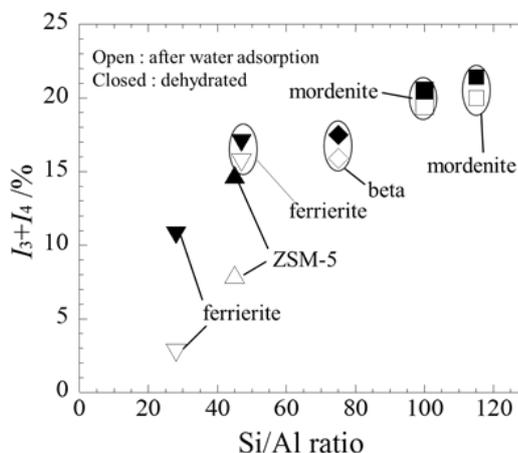
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Positronium(Ps) is a powerful probe for investigating pores with 0.2-1.0 nm diameter in porous materials. Zeolite is a porous material with regular tubular pores (0.4-0.8 nm diameter) and cavities with the basic unit of tetrahedral (SiO₄)⁴⁻ and (AlO₄)⁵⁻. There are various crystal structures, and chemical properties such as catalytic activity and ion exchange species change with different Si/Al ratios as well as crystal structures. Therefore, the chemical state of the surroundings of the tubular pores significantly affects the properties of zeolites. In this study, we have measured the Ps behavior, such as lifetime and formation rate, and correlated them with the crystal structure and the Si/Al ratio systematically.

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

The adsorption of water in the zeolite led to a decrease in the τ_3 lifetime and it was well correlated with the diameter of the tubular pores (Fig.1). The adsorbed water in the tubular pores hindered the diffusion of Ps, so that the *o*-Ps lifetime actually reflected the diameter of the pores with adsorbed water. We concluded that Ps can more easily diffuse in the cavities by dehydration and thus the *o*-Ps lifetime becomes longer. An increase in Al³⁺ ions gives rise to an addition of polar groups in the tubular pores. The plot of the sum of I₃ and I₄ vs Si/Al ratio is shown in Fig. 2. The higher the Si/Al ratio, the larger is the Ps formation component. Furthermore, water adsorption led to a decrease of the Ps formation intensity. This result was expected as electrons and positrons tend to be captured by the adsorbed water, leading to a decrease of the Ps formation probability.

Fig. 1 Plot of τ_3 vs diameter of tubular pores.Fig. 2 Plot of I_3+I_4 vs Si/Al ratio.

Change in Free Volume in Strained Rubber with Carbon Black Filler by *in situ* Positron Annihilation Lifetime Spectroscopy

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Tires are mainly composed of natural rubber, and various additives such as carbon black (CB) are added to increase the strength of the rubber. Especially CB, which is dispersed in the rubber, plays an important role to remarkably improve its mechanical properties. This reinforcing effect is thought to be related to the CB network, in which CB particles are connected to each other within a 3-nm thick layer, the so-called bound rubber, at the CB/rubber interface [1]. The detailed reinforcement mechanism is still unknown. In this study, we aimed to investigate the change in free volume within strained rubber with various amounts of carbon black filler by *in situ* positron annihilation lifetime spectroscopy (PALS).

The rubber consisted of isoprene rubber (IR) filled with various amount of CB (N330). The rubber specimens were prepared by mixing IR, CB and 1 phr (phr: parts by weight per 100 parts by weight of rubber) DCP (dicumyl peroxide) as the crosslinking agent. The CB content was varied from 0 to 80 phr. The rubber samples were strained to various strain ratios with a tensile tester and *in situ* PALS measurements were carried out. A ²²Na source was sandwiched within the strained samples and a 0.5 mm-thick Si wafer, in which Ps cannot form. Almost half of the positrons annihilated in the Si wafer and the other half in the strained sample, so that Ps formed only in the strained samples.

The o-Ps lifetime dependence on the CB content showed a minimum at 40 phr and generally no large changes were observed. The o-Ps lifetime dependence on the CB content was very similar to the dependence of the branch chain fraction of the CB network structure (number of branched chains / (number of branched chains + number of crosslinked chains)) on the CB content [1]. The o-Ps lifetime of the strained samples was measured *in situ*.

The o-Ps lifetime of the strained rubber samples hardly changed compared to the unstrained samples. On the other hand, a decrease in the intensity of the o-Ps component was observed in almost all the strained samples. The maximum change was measured in the sample containing 40 phr CB (Fig.1) and the minimum change was measured in the sample containing 0 phr CB. After releasing the sample, the intensity recovered. It is believed that the molecular chains in the amorphous phase become aligned when subject to tensile stress, thus leading to a decrease in the Ps formation.

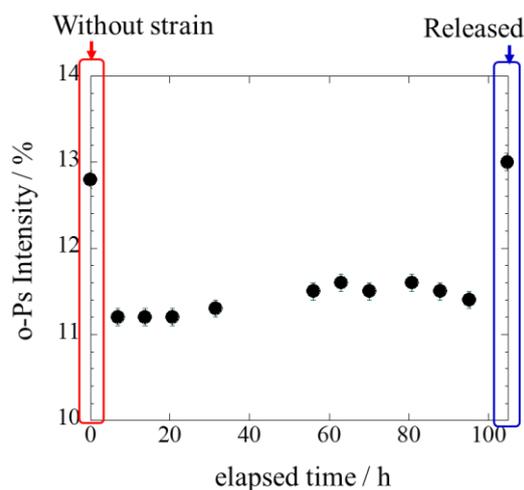


Fig.1. o-Ps intensity dependence of elapsed time in the sample 40 phr CB

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

Natural ageing and early precipitation stages in Al-Si-Mg alloys studied by positron annihilation spectroscopy

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Microstructure development during natural and artificial ageing of Al-Mg-Si alloys was studied employing positron annihilation spectroscopy (PAS) combined with transmission electron microscopy, electrical resistometry and microhardness testing. Solution treated Al-Mg-Si alloys contains Si-rich solute clusters and vacancies associated with Si solutes. This is in accordance with *ab-initio* theoretical calculations which revealed that vacancies are attracted to Si solutes but not to Mg ones. During natural ageing the concentration of vacancies gradually decreases and the solute clusters are enriched in Mg which was demonstrated by coincidence Doppler broadening. Combining electrical resistivity, hardness and PAS data enabled us to analyze the kinetics of the solute cluster development in various stages of natural ageing using the Johnson-Mehl-Avrami-Kolmogorov (JMAK) equation. The reaction order $\eta \approx 1$ determined in the stage III attributed to formation of defected Si,Mg co-clusters suggests diffusion-rate limited two dimensional growth. The reaction order $\eta \approx 2$ obtained in the stage IV associated with the development of vacancy-free Si, Mg co-clusters indicates interface-controlled transformation.

Peak hardening in artificially aged Al-Mg-Si alloys is caused by fine needles of the β'' phase. Results of positron lifetime spectroscopy combined with *ab-initio* theoretical calculations revealed that the composition of the β'' phase is $Mg_5Al_2Si_4$, i.e. it contains not only Mg and Si solutes but also Al atoms. Natural ageing has negative effect on artificial ageing since the composition of solute clusters formed during natural ageing differs too much from the composition of the β'' phase, namely the Mg content in solute clusters is too low. As a consequence β'' particles cannot develop from the solute clusters and β'' phase precipitation in the naturally aged alloys is retarded in comparison to solution treated alloys.

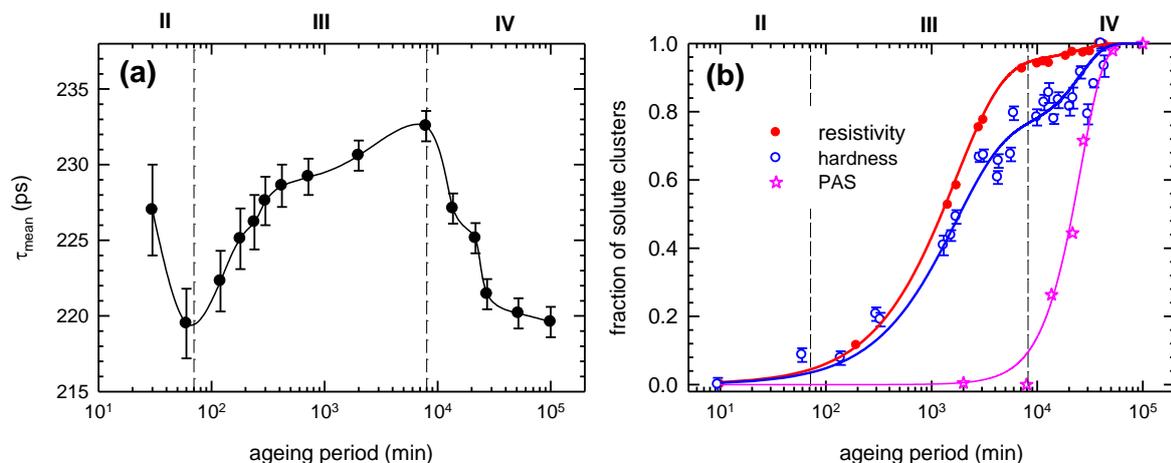


Fig. 1: Natural ageing of AlMgSiMnScZr alloy: (a) the development of the mean positron lifetime; (b) normalized fraction of developed solute clusters obtained from electrical resistometry, hardness and PAS measurements. Solid lines represent model curves obtained by fitting the data using the JMAK equation. Roman numbers indicate various stages of natural ageing.

**A detailed atomic investigation of the clustering process
on a Friction-Stir-Welding simulated Al-Cu-Li(-Mg) alloy (AA2198) by
Positron Annihilation Spectroscopy, SAXS and DSC**

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Al-Cu-Li(-Mg) alloys find wide applications in aviation and aerospace technology due to the reduction of weight and their high strength at the same time. After rolling sheets of these alloys, a defined heat treatment, following the solution annealing, leads to the formation of mainly T1-precipitates (Al₂CuLi). These precipitates are highly efficient in blocking dislocation movements [1]. When these sheets are joined by Friction-Stir-Welding (FSW), temperatures occurring in the Weld-Nugget (WN) are close to the material's solution treatment temperature (490-510°C).

Hence, the T1-precipitates are completely dissolved in this region, which results in a significant hardness-drop of 25%. Obviously, only GP-zones/GPB-zones and CuMg-clusters of several Ångströms in size are formed directly after welding by diffusion processes not understood in detail, yet [2]. We followed the precipitation kinetics directly after the Friction-Stir-Welding process with Differential Scanning Calorimetry (DSC), giving information on formed precipitates by their dissolution signal, Small Angle X-ray Scattering (SAXS), giving information on type, size and density of precipitates, Vickers-Hardness and Positron Annihilation Lifetime Spectroscopy (PALS), being sensitive to vacancies and dislocations as well as to the formation and growth of precipitates. Therefore, a Welding-Simulator was developed to reproduce the temperature-profile in the welded material.

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Influence of highly diluted alloying elements on the formation of vacancies in aluminum

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Positron annihilation lifetime spectroscopy (PALS) is applied to study the point defects generated in aluminum alloys upon quenching. Aluminum alloy having 0.025 at % In is used in this study. The samples were homogenized for 2 h in the temperature range 320-620 °C, then rapidly quenched in ice water. They were immediately measured at room temperature (RT) by positron lifetime spectroscopy. The samples were isochronally annealed in the temperature range up to 327 °C in steps of 10 °C, they cooled down after each annealing step to RT and measured by PALS. It is found that the average positron lifetime increases to 240 ps with increasing quenching temperature up to 470 °C and it decreases slightly with further increase of the quenching temperature, as shown in figure 1. A reference pure aluminum (99.9995) samples is quenched at different temperature to show the influence of the alloying element on the vacancy formation. An average lifetime of 170, very close to the bulk value (158 ps), is obtained, indicating the role played by the alloying element (In) on the vacancy formation.

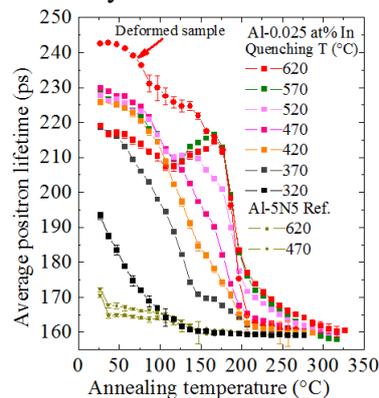


Fig. 1: Average positron lifetime as a function of the annealing temperature in Al-0.025 at% In alloy quenched at different temperatures.

Another sample is deformed to determine the positron lifetime in dislocations. The sample showed a defect lifetime of 242 ps, which is ascribed to the annihilation of positrons in dislocations. A defect-related lifetime of 247 ps is obtained in all quenched samples immediately after quenching. This lifetime corresponds mostly to vacancy-In complexes and dislocations. The defect-related lifetime is found to decrease with increasing annealing temperature up to 127 °C reaching 225 ps, then it increases reaching 280 ps, corresponding to divacancy. However, coincidence Doppler broadening spectroscopy is planned to be studied for these samples to get more information on the chemical surroundings of the observed defects. An activation energy for the vacancy-complex of 1.51 eV is determined from the positron lifetime data.

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**Vacancy Binding to Solute Atoms and Stability of Cu-Precipitation
in AlCu Alloys**

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We present first principle calculations on formation and binding energies for Cu and Zn as solute atoms forming small clusters up to 9 atoms in AlCu and AlZn alloys. The exact numbers are still under discussion since they are experimentally not easy to access and numerically there are still large uncertainties [1, 2]. We employ the density-functional approach implemented using projector-augmented waves and plane wave expansions as implemented in VASP, but also localized orbital as implemented in the code SIESTA. We find that some structures in which Cu atoms are closely packed on {100}- planes turn out to be extraordinary stable. We compare the results with existing numerical or experimental data when possible. We find that Cu atoms precipitating in the form of two- dimensional platelets on {100}-planes in the fcc aluminum are more stable than three-dimensional structures consisting of the same number of Cu-atoms. The preference turns out to be opposite for Zn in Al. Both observations are in agreement with experimental observations.

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Ageing Processes in the Aluminium Alloy AW6060 (Al-Mg-Si) Studied by Positron Annihilation and High-Precision Dilatometry

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Despite the great relevance of age hardenable aluminum alloys, the atomistic processes underlying the hardening process are not fully understood yet. In order to investigate the microscopic mechanism, in addition to techniques like electron microscopy, atom probe and difference scanning calorimetry, positron annihilation has been used for many years now.

In the present study, novel insight is gained by combining positron annihilation with high stability in-situ laser dilatometry. Dilatometric measurements were performed in a self-developed laser dilatometer with a rate resolution below 1nm/h [1,2]. While the present dilatometry technique opens up the pathway of direct monitoring of precipitation processes, positron annihilation yields additional insight into atomic defects and clusters involved in these processes. During artificial aging of the commercial aluminum alloy (Al-Mg-Si: EN-AW6060) on short timescales, a characteristic two step increase in the length change matches the variation of the mean positron lifetime giving hints on the early cluster formation process. Furthermore, the well-known aging characteristics of the hardness turned out to be directly related to the observed variations of dilatometric free volume and positron lifetime. These results show that dilatometry ideally complements positron annihilation.

Financial support by the Graz inter-university cooperation on natural sciences (NAWI Graz) is appreciated.

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Effect of Sn on the ageing kinetics of Al-Mg-Si alloys

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The influence of minor Sn additions on natural ageing (NA) in Al-Mg-Si alloys was studied by positron annihilation lifetime spectroscopy (PALS). From the perspective of vacancies, we found that in addition to the Sn content and solution heat treatment temperature, there are other factors which may directly or indirectly influence the retarding effect of Sn on solute clustering, including, but not limited to, the Mg and Si content as well as impurities such as Fe and Mn. The largest effect was observed in an Al-0.4Mg-0.4Si (at.%) alloy containing 70 ppm Sn and solutionised at 570 °C. By analysing activation energies deduced from one-component isothermal PALS ageing experiments at different temperatures and decomposing positron lifetime spectra into various components, we attempt to introduce some new concepts on the mechanisms of NA cluster formation in the presence of Sn by correlating various vacancy-solutes interactions with their diffusion kinetics.

Interaction between dislocations and impurities in strained aluminium by positron annihilation spectroscopy

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Aluminium and its alloys are widely used in construction, food packaging, gas containers, utensils and the automotive industry due to their light weight and high strength. However, pure Al has relatively low strength and unstable mechanical properties. In order to improve its mechanical properties, impurities can be added in the production process [1], which drastically improves its tensile strength [2]. In the solid-solution strengthening process, in particular, the hardening of aluminium occurs through the locking of dislocations around the solute atoms under plastic deformation. Nevertheless, the nature of those impurity atoms that inhibit the dislocation mobility has not been identified yet.

In this work, we investigated the behaviour of solute atoms around dislocations in strained alumina with different purities by positron annihilation lifetime spectroscopy. The samples were 1 mm-thick 5N and 2N Al that had been annealed at 580 °C for 1 h to remove defects and then subject to various tensile deformations until fracture at a strain rate of $5.5 \times 10^{-5} \text{ s}^{-1}$. The spectra measured at each strain value were fitted using two components, corresponding to the positron lifetime in the bulk and at the dislocations. A rise in the dislocation density with increasing strain was observed for both 5N and 2N Al, although the increase was about 4 times larger in the latter. The locking of the dislocations around the impurity atoms is considered the likely cause of this dislocation growth. The same samples were then analysed using coincidence Doppler broadening spectroscopy to identify the elements around the dislocations. No significant change in the shape of the CDB spectrum was detected in the strained 5N Al samples compared to the defect-free sample. This suggests no influence of the impurities on the dislocations in 5N Al. On the other hand, in the strained 2N Al samples a peak in the CDB spectra appeared as the deformation progressed (Fig. 1). This peak is believed to originate from the impurity atoms locked at the dislocations. In order to identify these elements, we also measured the CDB spectra of pure Fe and Si, which are the main impurities in 2N Al. The shape of the composed pure Si + Fe (8%) spectrum (Fig. 1) resembles very well that of the 2N Al spectrum. This indicates the formation of dislocation-Si and dislocation-Fe atom complexes in strained 2N Al.

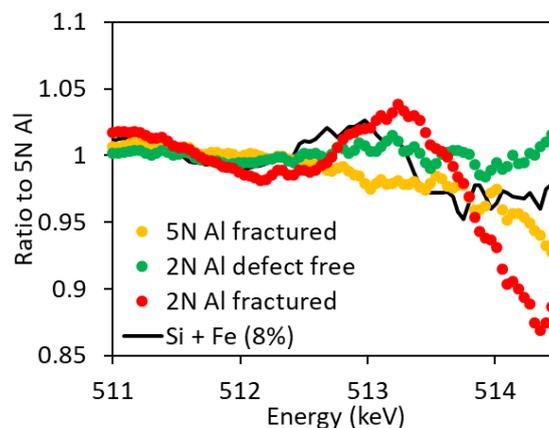


Fig. 1: CDB spectra of fractured 5N Al, defect-free and fractured 2N Al, and pure Si + Fe (8%).

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Silicon Quantum Dots in Silicon Nitride Formed by Solid State Precipitation

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Self-assembled silicon nanoparticles or quantum dots show promise as a light-emitter that is compatible with integrated circuit fabrication technologies. Si-QDs can be created by a variety of methods including Si implantation into SiO₂ films, and chemical vapour deposition of Si-rich silicon nitride films, followed by annealing. The process of solid-state precipitation of excess silicon to create QD's is not understood in detail, nor are the processes by which these structures emit light.

Structural aspects have been studied by ion beam, x-ray, and positron annihilation techniques, and optical properties by photoluminescence spectroscopy (both static and time-resolved). We have shown that vacancy-mediated diffusion plays a critical role in QD formation, and we expect this will be relevant to a range of nanostructural applications.

Computational study of correlation between local structures and positron annihilation parameters for cation vacancies in nitride semiconductor alloys

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Nitride semiconductors such as GaN attract increasing attention not only for applications in light-emitting devices but also for those in power devices. The alloying technique is often used to control the band gap. Since the positron annihilation S and W parameters are useful to identify defect species, we calculated these parameters for defect-free states, cation vacancies (V_C) and divacancies (V_2) in $\text{In}_{0.5}\text{Ga}_{0.5}\text{N}$ and $\text{Al}_{0.5}\text{Ga}_{0.5}\text{N}$ [1-3]. They were modelled as random alloys by the special quasirandom structure (SQS) approach [4]. Cation sites are not equivalent to each other and the calculated parameters for V_C and V_2 show distributions over finite ranges. Figure 1 represents the calculated S - W distributions. As usual, higher S values and lower W values were obtained for defects compared with those for the defect-free states. It is also noticeable that the S - W distribution for each defect shows a different form between two compounds.

In the present study, we have investigated the origin of the different distribution forms in terms of local atomic arrangements and electronic structures. In addition, calculations for larger defects such as V_C - nV_N ($n = 2, 3$) and for defects in $\text{Al}_{0.5}\text{In}_{0.5}\text{N}$ are ongoing. These results will be reported also. All the calculations have been performed using our computational code QMAS (Quantum Materials Simulator).

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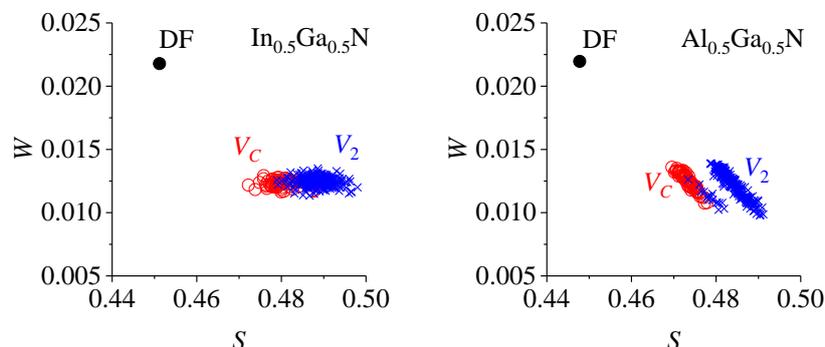


Fig. 1: Calculated positron annihilation S and W parameters for defect-free (DF) states, cation vacancies (V_C) and divacancies (V_2) in $\text{In}_{0.5}\text{Ga}_{0.5}\text{N}$ and $\text{Al}_{0.5}\text{Ga}_{0.5}\text{N}$.

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Study of Ion-Beam-Synthesized β -FeSi₂ Films probed by a Slow Positron Beam

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β -FeSi₂ is expected as an infrared-light receiving/emitting material replacing InGaAs since it does not contain rare metals or harmful elements [1]. Forming β -FeSi₂ in the surface layer of the Si substrate by annealing after implanting Fe ions into Si is called ion-beam synthesis (IBS) technique, and is well compatible with the Si-LSI process. However, the emission intensity is still insufficient for practical application. Terai and Maeda reported that the emission intensity of IBS β -FeSi₂ is enhanced by doping with Al atoms which occupy Si sites [2]. They claimed that the enhancement by Al-doping is caused by filling Si vacancies which act as nonradiative recombination centers. In this study, the undoped and Al-doped IBS β -FeSi₂ films were probed by a slow positron beam.

High-resistivity FZ-Si(100) substrates were implanted with a maximum energy of 100 keV Fe⁺ ions to a total dose of 1×10^{17} ions/cm² at room temperature. Al⁺ ions were additionally implanted as an Al-doped sample to a total dose of 5×10^{15} ions/cm² with a maximum energy of 50 keV. After the implantation, the substrates were annealed at 800°C for 2 hours in vacuum to synthesize the β -FeSi₂. According to the previous studies [1,3], the β -FeSi₂ layer is reported to be formed with a thickness of 50 nm at the surface of the Si substrate under these implantation and annealing conditions. The Doppler broadening of annihilation radiation (DBAR) spectra were acquired for both samples at room temperature with varying incident positron energies. All the samples were treated with dilute hydrofluoric acid to remove the native oxide film before the positron annihilation measurements.

Figure 1 shows S parameters for the undoped and Al-doped IBS β -FeSi₂ samples as a function of incident positron energy. The incident-energy region of 2–4 keV corresponds to the β -FeSi₂ layer. Larger S parameters are observed for the Al-doped β -FeSi₂ sample which is reported to show the enhanced emission intensity. This result, contrary to our initial expectation, suggests that more vacancies are introduced into the IBS β -FeSi₂ by the Al-doping. We consider that the formation of vacancy-Al defect complexes to reduce lattice strain caused by a large atomic radius of Al atoms is one possibility for the increase of S parameters.

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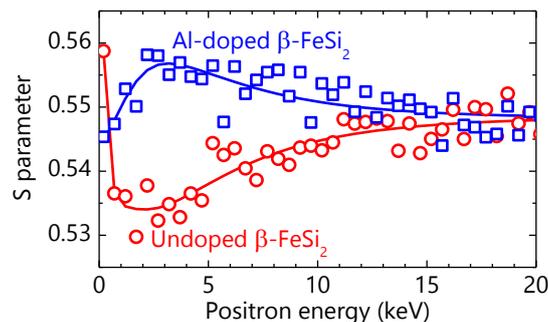


Fig. 1: S parameters for the undoped (open circles) and Al-doped (open squares) β -FeSi₂ samples.

Positron Annihilation Studies using a Superconducting Electron LINAC

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The Helmholtz-Center at Dresden-Rossendorf operates several user beamlines for materials research using positron annihilation energy and lifetime spectroscopy. Two beamlines are being operated at a superconducting electron linear accelerator [1] producing hard X-rays from electron-bremsstrahlung and in turn generating positrons from pair production. Both installations employ bunched continuous-wave (CW) electron beams with energies between 15 MeV and 30 MeV. The CW-operation results in significantly reduced pile-up effects in the detectors in comparison to normal conducting accelerators. Electron bunch lengths below 10 ps FWHM allow positron annihilation lifetime spectroscopy measurements with high timing resolutions. The bunch repetition rate is adjustable to $26 \text{ MHz} / 2^n$, $n=0, 1, 2 \dots 8$ matching wide spans in positron or positronium lifetimes. The Gamma-induced Positron Source GiPS generates energetic electron-positron pairs inside the sample under investigation from hard x-rays impinging onto the sample [2]. Therefore, the source is especially suited for materials which are not qualified for vacuum conditions or because they are imposing hazardous conditions or intrinsic radioactivity. Exemplary defect studies on the Skyrmion-lattice compound MnSi [3] will be presented. The Mono-energetic Positron Source MePS utilizes positrons with fixed energies ranging from 500 eV to 16 keV [4]. A magnetic beam transport system guides positrons to the samples under investigation. A dedicated chopper/buncher system is used to maintain a high timing resolution for depth-dependent annihilation lifetime studies in thin films. The signal-to-noise ratio is beyond 10^4 while lifetime resolutions of around 280 ps FWHM have been obtained. Applications of porosimetry studies in low-k dielectrics [5] and polymer brushes [6] will be presented.

The MePS facility will be extended by an end-station called AIDA2 (Apparatus for in-situ Defect Analysis) where defect studies can be performed in a wide temperature range during thin film growth and ion irradiation. A similar setup named AIDA-1 is already in operation at a ^{22}Na -based mono-energetic continuous positron beam [7] used for Doppler-broadening spectroscopy experiments [8,9].

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Defect Imaging Using the Positron-Microbeam of the CDB Spectrometer at NEPOMUC

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The Coincidence Doppler Broadening Spectrometer (CDBS) at the positron beam facility NEPOMUC was upgraded with a beam brightness enhancement system in order to enable CDB spectroscopy with improved spatial resolution. The positron is transported in a newly designed μ -metal shielded optically column comprising several electrostatic lenses, magnetic compensation coils, and beam monitors. A new piezo controlled positioning device allows spatially resolved defect spectroscopy by scanning the positron beam in an area of $19 \times 19 \text{ mm}^2$. The new brightness enhancing device is integrated in the electrostatic beam guiding system and basically comprises a beam focusing unit and a Ni(100) foil of 100 nm thickness working as transmission remoderator.

In order to achieve a high yield of re-emitted moderated positrons, the Ni foil can be heated to about 600°C in a H-atmosphere in order to remove surface contaminations such as C and O. Without remoderator the positron implantation energy can be varied between 0.2 and 30 keV. For higher spatial resolution the positron beam is first focused onto the thin single crystalline Ni remoderation foil before it is accelerated to up to 25 keV onto the sample.

In order to estimate the beam diameter at the sample position spatially resolved DB measurements have been performed on a special sample as shown in Fig.1 (a). The CDBS *upgrade* without remoderator yields a lateral resolution of $200 \mu\text{m}$ (FWHM) which is already an improvement of about 20% compared to the previous setup (Fig.1 (b,c)). By using the brightness enhanced beam, the beam spot could be further reduced by a factor of four, i.e. to $50 \mu\text{m}$ (FWHM); see Fig.1 (d). Benefiting from the improved resolution of the CDBS *upgrade*, defect spectroscopy on various light metal alloys has been performed recently.

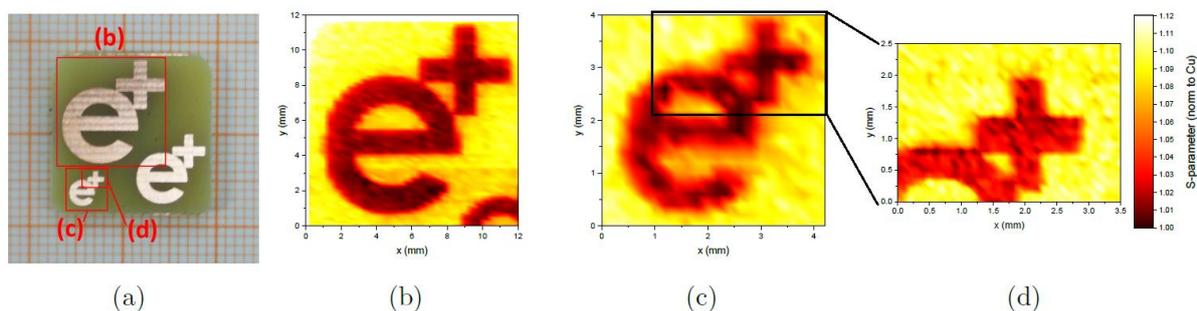


Fig. 1: 2D S-parameter maps of an etched copper e^+ pattern: (a) photo of specimen showing scanning areas; S-parameter maps scanned with (b, c) the re-moderated beam of NEPOMUC and with (d) the brightness enhanced beam after remoderation in the CDB spectrometer *upgrade*.

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Novel Reflection High-Energy Positron Diffractometer at NEPOMUC

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The arrangement of topmost atoms determines fundamental physical processes at surfaces such as de- and adsorption, diffusion or chemical reactions. Therefore, the precise knowledge of the surface structure is essential to e.g. calculate the electronic structure, optimize catalytic techniques or develop nanoelectronic devices. It has been shown that Total Reflection High-Energy Positron Diffraction (TRHEPD) is a powerful tool to determine atomic positions of topmost layers and hence surface structures with unprecedented accuracy [1]. In contrast to its electron counterpart, Reflection High-Energy Electron Diffraction (RHEED), positrons are repelled from the crystal surface and exhibit the phenomenon of total reflection when the glancing angle is smaller than the critical angle θ_c .

Currently, we develop a new TRHEPD setup coupled to the high-intensity positron source NEPOMUC, located at the research reactor FRM II in Munich. Since the NEPOMUC beam provides an intensity of 10^9 moderated positrons per second [2], we expect a further reduction of the measurement time and improved statistics using the new TRHEPD setup. A cross-sectional view through the measurement plane is shown in figure 1. The TRHEPD setup features UHV down to 10^{-10} mbar, sample temperatures up to 800°C , a Faraday cage to shield electrostatic fields and a RHEED system for complementary measurements.

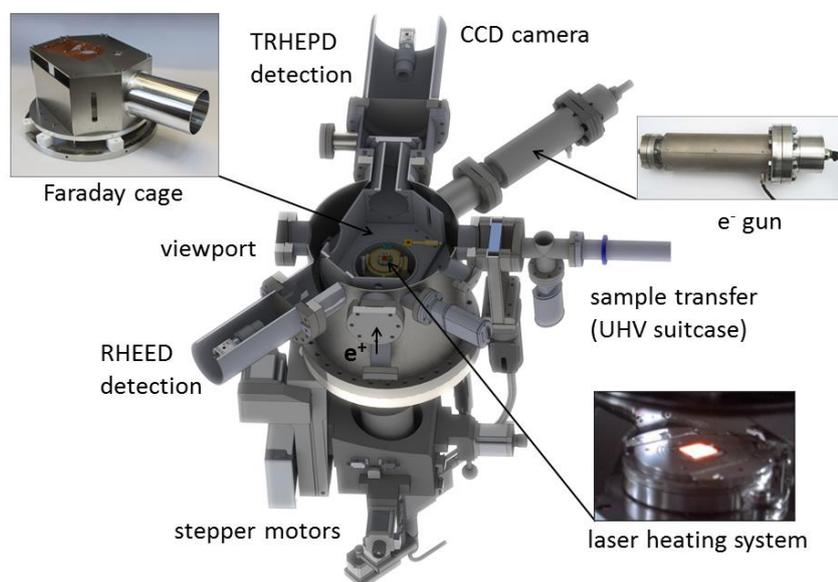


Fig. 1: Cross-sectional view through the measurement plane of the TRHEPD UHV chamber.

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The estimation of positron production and heat generation in KUR beam line by PHITS

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In recent years, the requirement of strong positron beam has increased. Variable energy positron beams enable depth distribution analysis of vacancy-type defects in materials. The Kyoto University Research Reactor (KUR) is a light-water-moderated tank-type reactor operating at a maximum thermal power of 5 MW. In order to promote the research application of the KUR, a high-intensity positron beam line has been designed and constructed.

There is a strong motivation for improving the beam line, especially the positron beam intensity. For this purpose, the optimization of the converter and moderator is necessary. In this study, the positron generation behavior in the KUR positron beam line is simulated by using the Particle and Heavy Ion Transport code System (PHITS). The PHITS is a general purpose Monte Carlo particle transport code. It deals with the transport of particles such as nucleons, nuclei, mesons, photons, electrons and positrons over wide energy ranges, using several nuclear reaction models and nuclear data libraries. Geometrical configuration of the targets is possible to set. Various quantities such as heat deposition, track length and production yields of each particle is obtained from the simulation. In this calculation, the input file of the code contains the neutron spectrum, the gamma ray spectrum and geometry of converter. For the increase of gamma rays and the shielding of neutrons from the reactor core, a 1 mm thick Cd plate was used. The thickness of W converter is 1 mm and the distance between Cd and W plates is 10 mm.

Table 1 shows the calculated results. ‘ γ -ray, 0 cm’ means only the contribution of γ -rays coming directly from the reactor core at the end position of irradiation hole. ‘30 cm’ is the present position of the W converter which is 30 cm inside from the end of the hole. ‘n+Cd’ means the production of positrons only by the contribution of neutrons with $^{113}\text{Cd}(n, \gamma)^{114}\text{Cd}$ reaction. The generation of positrons by γ -rays with neutrons and Cd plate is almost the same at 0 cm but small at 30 cm compared to that by γ -rays directly from the reactor core. The deposition of energy is also important because the beam tube is made of Al and the mechanical property decreases at high temperatures. The deposition energy of positron production with neutrons and Cd plate is by 3 (0 cm) and 12 (30 cm) times higher than that with no Cd plate.

Table 1: The generation of positrons and deposition energy calculated by the PHITS code

Incident Particles	Positron generation rate (e ⁺ /cm ² /s)	Total deposition energy (MeV/s)
γ -ray, 0 cm	1.47×10^9	1.10×10^{12}
γ -ray, 30cm	1.18×10^8	8.80×10^{10}
n+Cd, 0 cm	1.30×10^9	3.27×10^{12}
n+Cd, 30 cm	4.02×10^8	1.02×10^{12}

Application of LYSO scintillators in positron annihilation spectroscopy

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Lutetium-yttrium oxyorthosilicate (LYSO) scintillator offers high stopping power, fast bright scintillation and high light output. These parameters are crucial when it comes to fast timing detection as by positron annihilation life-time spectroscopy. It has been proven, that same size LYSO scintillator provides higher detection efficiency than widely used BaF₂, but its time resolution decreases [1], [2], [3]. However, according to [3], the time resolution can be improved by using of small sized LYSO crystals keeping count rate at the same level as when using of BaF₂ scintillator. The system time resolution FWHM of about 193 ps and the coincidence counting rate 8 cps/μCi were achieved by Dao-Wu with two detector layout [3].

The aim of this paper is to find optimal dimensions for LYSO crystal with application in positron annihilation life-time spectroscopy using Geant4 simulation toolkit. The Geant4 simulation allows to estimate an influence of the measuring geometry on detection efficiency and to choose the most appropriate crystals dimensions and source to detector positions. Application in 3 detector layout is investigated and possible geometry is suggested.

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Digital data acquisition for positron lifetime measurements

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For over 10 years of research the positron group at the Martin-Luther-University Halle-Wittenberg successfully employed a digital positron lifetime setup using an Agilent digitizer connected to two Hamamatsu photomultipliers with plastic scintillators, inhouse built high-voltage sources and coincidence trigger units. Collected data are analyzed online with a software written in C++ using a graphical user interface designed with QT. Right now, five stations are in operation; four setups with two detectors like the common analog setups and one setup using four detectors in parallel. The four-detector-setup enables measurements with a large solid angle at high count-rates. It is possible to measure 10^6 annihilation events in less than ten minutes or 10^5 in one minute, which allows studying slow dynamic processes like thermal annealing of metal samples. The data analysis is done using recorded waveforms of photomultiplier anode pulses by calculating the pulse maximum with a cubic spline interpolation in a defined array both around the recorded maximum and the raw constant fraction array at 30% of the pulse rising edge yielding an improved maximum and timestamp for each pulse [1]. After all, the lifetime is calculated as the time difference between the two timestamps of two detectors. Both photomultiplier can be used as start and stop by individually selected gates and thus increasing the number of usable events.

After the measurement, the spectra are summed. By improving the positron lifetime time calculation with the digital data acquisition an average time resolution of 170 ps FWHM could be achieved, which is 30 ps better than an equivalent analog system. The influence of sampling-rate, bandwidth and digital resolution will be presented. The best resolution of 130 ps FWHM were obtained by using the optimal settings in combination with a small plastic scintillator. The limits of the digital measurement are caused by a huge amount of useless data before and after the pulse, which is needed for long lifetime measurements with an external trigger (a digital dataset of 1000 ns by 2GS/s accounts for 2000 points per channel per pulse) causing a significant bandwidth limit. To reduce the number of collected data traffic an online FPGA pulse detection and analysis firmware within a SPDevices digitizer has recently been implemented which filters only the useful part around the pulses and send only this reduced dataset (with an extra timestamp header) to the computer. The pulse detection option generates a single trigger event for each channel if the pulse crosses the analog threshold and only a few points before and after this trigger event were stored. With this feature, it is possible to work with a count rate up to 110k counts per second, which is helpful to implement the digital acquisition at systems like MePS [2] or GiPS [3] at the HZDR without losing a big part of the data while the data transfer time.

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Positron lifetime triple coincidence filtering

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The three-detector positron lifetime spectrometer is often used technique in investigation of materials containing disturbing radioactive ^{60}Co source. Triple coincidence is a solution to suppress this unwanted contribution to lifetime spectra. With digital setups, the second advantage of the three detector setups is the possibility to average two measured lifetimes from one annihilation event which contributes to improvement of the PALS time resolution. In this article a filtering technique, like coincidence doppler broadening of the annihilation energy filtering is described.

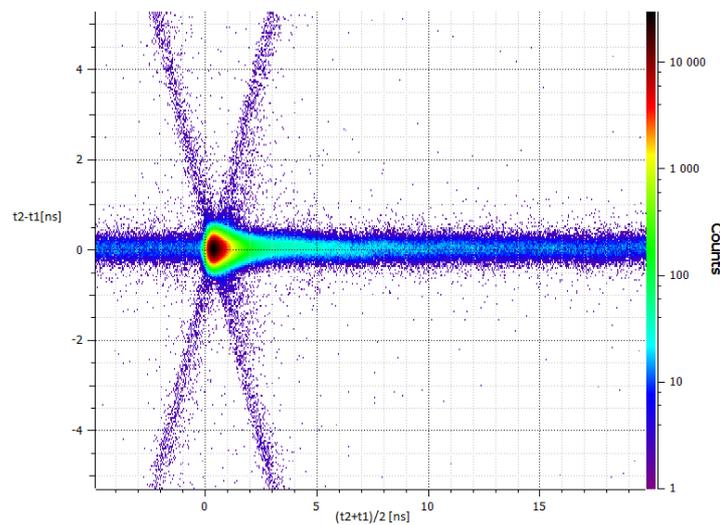


Fig. 1: 2D histogram based on two simultaneous positron lifetime measurements in triple coincidence.

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Positron Emission Tomography - an introduction and overview about current developments

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Positron Emission Tomography (PET) is a quantitative functional imaging technique in nuclear medicine that is applied in oncology, neurology and cardiology for more than 40 years. Ongoing developments in PET detector technology and image reconstruction lead to a tremendous improvement in the reconstructed PET image quality. Moreover, the combination of PET with CT and MRI scanners in the last years enabled true hybrid imaging that combines high-resolution anatomical and functional imaging.

This talk gives an introduction into the principles of PET imaging and provides an overview about the latest developments in PET image reconstruction and PET detector technology.

Slow positron beam spectroscopy study of PMMA nanocomposite films with ion-synthesized silver nanoparticles

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Understanding how the size, shape, and the aggregation state of the silver nanoparticles (NPs) are changed after integration into a target matrix is critical to enhance their performance, including molecular diagnostics, photonic and biomedical devices, which take advantage of the novel optical properties of these nanomaterials. In particular, the nanocomposites containing noble metal NPs dispersed in the polymer matrix by high-dose ($> 10^{16}$ ions/cm²) implantation at low-energy ions (< 100 keV) can be used for the construction of plasmonic waveguides [1] and diffraction gratings [2]. Typically, form and size of Ag NPs in optically transparent matrices are connected with an appearance in visible absorption spectra of composite a surface plasmon resonance band. However, synthesis of Ag NPs by ion implantation in transparent polymer matrix such as polymethylmethacrylate (PMMA) has been found [1] to be quite difficult and unusual.

This problem can be solved with a powerful technique for the characterization of thin films – positron annihilation spectroscopy (PAS) using a variable-energy positron beam (VEPAS), – allowing depth-profiles from tens of nanometers up to several micrometers. This technique has been emerged as a key experimental tool for the understanding high-dose 40 keV boron-ion-implanted polymethylmethacrylate (B:PMMA) [3] with carbon nanostructures and Ag NPs loaded polymer brushes [4]. Also, the first attempt to find difference between the effects of carbonization and formation of Ag NPs in high-dose B:PMMA and Ag:PMMA nanocomposites has been done in the work [5] by using the Doppler broadening slow positron beam spectroscopy (DB-SPBS).

In the present work, the DB-SPBS technique was applied to characterize further the 30 keV Ag:PMMA nanocomposites fabricated by low-energy high-dose Ag-ion implantation. The results of depth profile of the $S(E_p)$ parameter in the near-surface region of irradiated polymer were used to clarify indirectly a formation of Ag NPs in PMMA in dependence on ion dose. By comparative analysis with the $S(E_p)$ parameter trend in polymer brushes with loaded Ag NPs [4], it is found that the density or mass of Ag NPs ('Ag filling') in Ag:PMMA increases as ion dose grows. The results obtained are discussed in terms of the positronium formation fraction in the irradiated part of polymer matrix and the model of carbon-shell Ag-core nanoparticles.

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Positron Annihilation Spectroscopy for the study of polymer brushes

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Positron Annihilation Spectroscopy (PAS) has recently been applied by our Group for the first time to characterize nanoparticle-loaded polymer brushes and gel-brushes [1-3], which are at the core of many innovative devices [4].

Polymer brushes were obtained by means of the grafting-from technique, i.e. the polymer chains were grown directly from an initiator-functionalized surface. Brush-gels are crosslinked systems obtained polymerizing both a mono- and a difunctional monomer. Subsequently, nanoparticles (in this case, silver nanoparticles) could be either loaded or synthesized *in situ* [1,3]. The control over nanoparticle distribution and the polymer brushes structure is crucial and, in order to gain sufficient insight, the use of arrays of different techniques is typically required.

We adopted Doppler Broadening Spectroscopy (DBS) to investigate, in a non-destructive way, the infiltration of silver nanoparticles within polymer brushes and brush-gels and we were able to obtain an estimation of the number density of Ag nanoparticles infiltrated between the polymer chains. Moreover, we demonstrated that unprecedented details about the influence of the initiator on the structure of the polymer brushes were obtained from Positron Annihilation Lifetime Spectroscopy (PALS) measurements.

The goal of the present work is to give a detailed account on the versatility of PAS for the study of polymer brushes, brush-gels and of their composites with nanoparticles.

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Development of self-standing mesoporous thin films for positronium formation in transmission

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Transferable mesoporous silica thin films (thicknesses between 740-760nm) were developed as a new step towards low-energy Positronium (Ps) formation in the transmission geometry. The films were characterized via a variable energy positron beam with a 0.1-20 keV range. For positron implantation energies (~1 keV), the ortho-Ps (o-Ps) formation yield was estimated to be ~65% via the three-gamma method. From simulations, formation of Ps in the transmission geometry is predicted to allow a higher quantity cold o-Ps emitted into vacuum [1]. Lifetime measurements were undertaken to determine the pore diameter (3-4 nm) and o-Ps emitted into vacuum.

A sol-gel mixture of TEOS ($\text{Si}(\text{OC}_2\text{H}_5)_4$), water (pH=1.25 with HCl) and ethanol to a molar ratio of (1:5:3.8) based on [2], was prepared. A cationic surfactant (CTAB: $\text{CH}_3(\text{CH}_2)_{15}\text{N}^+(\text{CH}_3)_3\text{Br}^-$) was added to 0.1 CTAB/Si molar ratio and then diluted with ethanol (ratio 1:1). The sol-gel was spin-coated onto a Si (111) substrate. Calcination was undertaken for thorough removal of the organic components, leaving a mesoporous silica thin film. The self-standing films were created by spin-coating a base layer of polystyrene/toluene solution [3], original sol-gel recipe spin-coated on top, then allow the thin film to be released via the dissolution of the polystyrene layer. This film was transferred to a holed substrate with a transmission of ~69%, produced by femtosecond laser irradiation, followed by chemical etching [4].

The internal nanostructure was determined to have a disordered, worm-like structure with differing morphology at the bulk-air and bulk-substrate interfaces, based on XRD and HRTEM results.

This is a large step toward the realisation of a self-standing target capable of producing high quantities of cold o-Ps into vacuum in the transmission geometry. The AEGIS (Antimatter Experiment: Gravity, Interferometry, Spectroscopy) collaboration plans to exploit this increased quantity of cold Ps for antihydrogen formation via charge exchange [5]. This also opens the feasibility for future Positronium Interferometry experiments [6].

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Configurations of Point Defects in Float-Zone n-Type Silicon Irradiated By 0.9-MeV Electrons and 15-MeV Protons

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We will focus on the atomic configurations and thermal stability of the vacancy defects involving Group-V-impurity atoms in silicon. The discussion is centered on the phosphorus-vacancy complexes which for several decades have been elusive for observation.

The emphasis will be placed on Group-V-impurity-atom vacancy complexes of radiation origin in oxygen- and carbon-lean float-zone silicon single crystals. In order to probe the open vacancy volume of defects (V_{op}) in the course of their isochronal annealing we used the low-temperature positron annihilation lifetime spectroscopy (PALS). In order to amplify the positron annihilation data and to characterize the materials, low-temperature Hall effect has been studied. The samples used in experiments were cut from the same wafer.

It is argued that D_{3d} symmetry underlies configuration of thermally stable Group-V-impurity-atom $-V_{op}$ complex in the crystal lattice of the moderately doped silicon of n-type.

The open vacancy volume of thermally stable complex corresponds to the characteristic positron lifetime which ranges ~ 267 ps to ~ 298 ps. Theoretical values available for isolated vacancy and for a divacancy in silicon are in the same range of the positron lifetimes, thus suggesting that the open vacancy volume of Group-V-impurity-atom- V_{op} complex comprises, at least, a vacancy in the electron-irradiated material [1].

A role of the chemical nature of Group-V-impurity atom in forming the microstructure possessing D_{3d} symmetry is discussed in the light of data obtained for the volumetric atom of bismuth in bismuth-vacancy complex, Bi- V_{op} . Owing to the lattice deformation, which depends on the elemental specificity of Group-V-impurity atom involved in the complex, the symmetry D_{3d} may be changed (e. g. to O_h one); some predictions and examples of such possibility are presented.

As a result of comparative analysis of data of Hall effect and positron annihilation lifetime measurements, the configurations of the phosphorus-vacancy complex which involve one and two impurity atoms of phosphorus, P- V_{op} and P- V_{op} -P, are proposed.

These defects begin to decompose slowly at the isochronal annealing temperature ~ 300 – 350 °C. In the course of PAL measurements they had been observed up to ~ 500 – 560 °C. The decomposition of these phosphorus-vacancy complexes results in restoring the shallow donor states of the phosphorus impurity atoms. This restoration is observed up to the annealing temperature ~ 600 – 650 °C for the both electron- and proton-irradiated n-FZ-Si(P) materials.

It is argued that the couples of relaxed vacancies (or semi-vacancies) are involved in the open vacancy volume of P- V_{op} complexes. A similarity and distinctions in behaviour of these defects will be discussed for both electron- and proton-irradiated materials.

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Poster	First Author	Poster Title	Page
P1	J. Kuriplach <i>Charles University Prague, Czech Republic</i>	Defects in High Entropy HfNbTaTiZr Alloys Studied with Positrons	p. 76
P2	F. Lukac <i>Institute of Plasma Physics/ Charles University Prague, Czech Republic</i>	Defects in high entropy alloy HfNbTaTiZr prepared by spark plasma sintering	p. 77
P3	O. Melikhova <i>Charles University Prague, Czech Republic</i>	Hydrogen-induced defects in Ti and their thermal stability	p. 78
P4	V.S.M. Pereira <i>Delft University of Technology, Netherlands</i>	Doppler Broadening analysis of defect evolution in Eurofer97 and ODS Eurofer97 after He-implantation and annealing treatments	p. 79
P5	G.M.Tanzi <i>Università degli Studi di Milano, Italy</i>	A two-particle model for Positronium confined in sub-nanometric cavities	p. 80
P6	M. Elsayed <i>University Halle, Germany/ Minia University, Egypt</i>	Identification of defects in high-entropy alloys by positron annihilation spectroscopy	p. 81
P7	C. Naidoo <i>iThemba LABS, South Africa</i>	Improvements in the Production of ^{22}Na Positron Sources at iThemba LABS	p. 82
P8	R.S. Laptev <i>National Research Tomsk Polytechnic University, Russia</i>	Positron Spectroscopy of Intermetallic Hydrogen Storage Alloys Synthesis Based on Ti-Cr with C14 and C36 Laves Phases	p. 83
P9	A.M. Lider <i>National Research Tomsk Polytechnic University, Russia</i>	Positron Spectroscopy of Defect Structure Additively Manufactured Titanium Ti-6Al-4V	p. 84
P10	R. Krause-Rehberg <i>University Halle, Germany</i>	Improvement of depth resolution of VEPAS by a simultaneous sputtering technique	p. 85

Defects in High Entropy HfNbTaTiZr Alloys Studied with Positrons

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High entropy alloys (HEAs) – called sometimes “materials cocktails” – are a class of new materials based on many (at least four or five) constituting metals mixed in equimolar concentrations. Important characteristics of these alloys are their large configurational entropy and a single, simple phase they exhibit. HEAs are nowadays frequently studied because of their interesting properties. HfNbTaTiZr alloys were introduced recently [1] as a candidate to replace current materials in high temperature applications (all involved metals are refractories), and biocompatible applications are also envisaged. Since the defects’ structure, behavior and influence on HfNbTaTiZr alloys’ properties are largely unknown, we bring here first information. At the beginning, we investigate theoretically the alloy structure stability, short range order and behavior of vacancies. In particular, we address the question of existence of structural vacancies. Theoretical considerations presented in [2] suggest that structural vacancies do not exist in HEAs, but our *ab initio* calculations give some indications that such vacancies could be found.

On the experimental side, the HfNbTaTiZr alloy studied was prepared by vacuum arc melting of corresponding pure metals (purity 99.9 %) in a water cooled copper crucible. Each element was added to the melt in equimolar proportion. The casting was performed six times and flipped for each melt to mix the elements thoroughly and suppress chemical heterogeneity. The X-ray diffraction phase analysis revealed that the cast sample is a single phase with the bcc structure and lattice parameter $a = 3.4089(1)$ Å. Positron annihilation studies were performed using a digital positron lifetime (LT) spectrometer with the time resolution 144 ps and a digital coincidence Doppler spectrometer equipped with two HPGe detectors. The as-cast sample exhibits a two component LT spectrum. The shorter LT component comes from free positrons whereas the longer one with a lifetime of 165(1) ps represents a contribution from positrons trapped at defects. The defect component with an intensity of 94 % is dominating in the LT spectra of the as-cast sample. Annealing at 1000 °C for 1h caused a decrease in the intensity of the defect component indicating a partial recovery of defects. The theoretical bulk lifetime of HfNbTaTiZr alloys was estimated to be 142 ps from several fully relaxed model supercells using a parameter-free gradient-correction approach to electron-positron correlations [3]. Further calculations for various vacancy configurations are in progress, and their corresponding positron lifetimes will be compared to experimentally found LT components.

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Defects in high entropy alloy HfNbTaTiZr prepared by spark plasma sintering

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High entropy alloys exhibit various combinations of interesting physical properties due to the formation of solid solution stabilized by high configurational entropy. High entropy alloy HfNbTaTiZr exhibits single phase solid solution with BCC structure when prepared by arc melting [1]. Grain refinement achieved in cold rolled samples after recrystallization remarkably enhanced ductility of this alloy [2]. Mechanical alloying by milling and subsequent sintering is a frequent production way of preparing fine grained alloys from chemical elements with high melting temperature. In addition, spark plasma sintering (SPS) method with applied pressure serves as a unique tool of powder metallurgy thanks to fast heating rates and low time of exposition to elevated temperatures. Therefore, the deformation energy introduced during mechanical alloying may be effectively consumed during short sintering process and presents the additional parameter for grain refinement. The present work presents characterization of HfNbTaTiZr alloy prepared by SPS.

Microstructure of samples prepared by SPS was compared with as cast ingots. The samples were characterized by X-ray diffraction and scanning electron microscopy. Positron annihilation spectroscopy was employed for characterization of defects introduced by SPS and their thermal stability.

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Hydrogen-induced defects in Ti and their thermal stability

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Titanium readily absorbs hydrogen and undergoes phase transition into the hydride phase (TiH₂). In the hydride phase Ti is able to absorb the hydrogen concentration as high as 1.4 wt.%. These properties make Ti and Ti-based alloys attractive for hydrogen storage applications. Hydrogen absorption in titanium matrix may introduce open volume defects since the volume of TiH₂ phase exceeds that of titanium matrix. Absorbed hydrogen may segregate at these defects forming defect-hydrogen complexes.

In the present work positron annihilation spectroscopy was employed for characterization of hydrogen-induced defects in titanium. Defects created by hydrogen loading from the gas phase were compared with those introduced by electrochemical hydrogen charging. In general hydrogen loading introduces a high density of dislocations and vacancy clusters created by agglomeration of hydrogen-induced vacancies. The mean size of vacancy clusters depends on the hydrogen absorption temperature.

Thermal stability of hydrogen absorbed in titanium and recovery of hydrogen-induced defects were studied by positron lifetime spectroscopy combined with *in-situ* X-ray diffraction and thermal desorption spectroscopy. Fig. 1 shows the temperature dependence of positron lifetimes and relative intensities of individual components for hydrogen gas loaded titanium. The decomposition of TiH₂ phase is accompanied with introduction of additional vacancies agglomerating into vacancy clusters. Further annealing of the sample above 500 °C leads to recovery of dislocations.

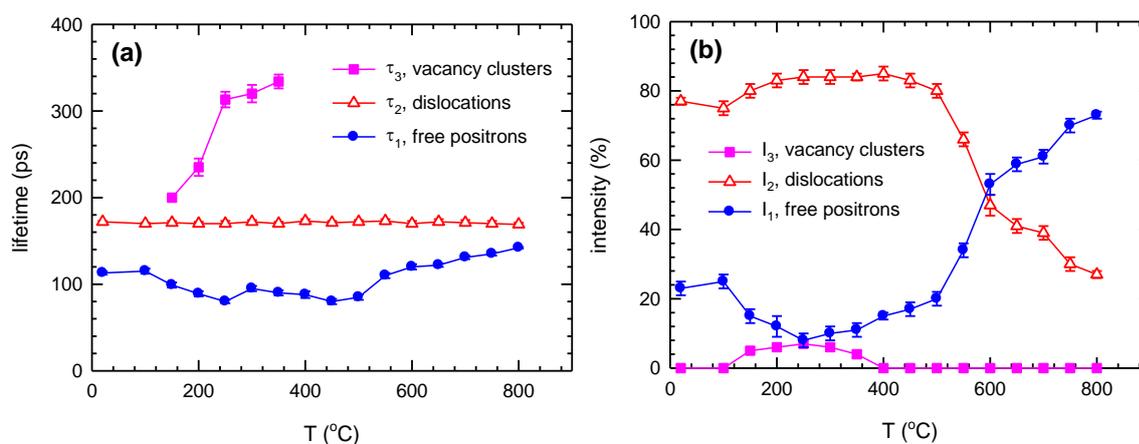


Fig. 1: Results of positron lifetime investigations of hydrogen loaded Ti (H₂ gas pressure 1 bar, temperature 400 °C): the development of (a) positron lifetimes and (b) corresponding relative intensities on the annealing temperature.

Doppler Broadening analysis of defect evolution in Eurofer97 and ODS Eurofer97 after He-implantation and annealing treatments

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The addition of nanosized Y₂O₃ particles in steels for nuclear fusion reactors is a new approach to improve performance at high temperatures (650-700 °C) and also to increase radiation damage resistance; however, the role of oxide nanoparticles is still not fully understood. In the present work, the formation and evolution of defects in Eurofer97 and Oxide Dispersion Strengthened (ODS) Eurofer97 alloys, after He implantation and at different working temperatures, is investigated. Samples of the two steels were He-implanted at room temperature, with 350 keV He ions and a dose of 10¹⁶ He ions.cm⁻². Then, the formation of defects in both steels was studied by Positron Annihilation Spectroscopy Doppler Broadening (PASDB), first at ambient temperature (23 °C) and then *in situ*, during annealing at temperatures up to 1200 °C (Eurofer97) and 1300 °C (ODS Eurofer97). The annealing treatments were made under a pressure of 10⁻⁷ mbar; the samples were heated gradually, with steps of 100 °C and duration of 5 min. At the end of each heating step and after cooling inside the furnace, the defect evolution was measured with PASDB.

The influence of the Y₂O₃ nanoparticles can primarily be observed by an increase in stability of voids in the ODS Eurofer97 steel. At critical temperatures – at which abrupt changes of state in defects take place – these more stable voids minimize undesired effects, such as volumetric expansion or embrittlement. These critical temperatures are 200 °C and 800 °C, which is in accordance with previous studies conducted on the same materials. The effect of He implantation doses, in comparison to previous studies with different doses, is highly influential on complex cluster formation and on triggering helium release mechanisms. An implantation dose of 10¹⁵ He ions.cm⁻² is required to observe the significance of He bubbles in high He concentration regions in Eurofer97, while from implantation doses of 10¹⁶ He ions.cm⁻² onwards, also low He concentration regions will undergo complex cluster formation.

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

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

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

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

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

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Identification of defects in high-entropy alloys by positron annihilation spectroscopy

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High-entropy alloys (HEAs) have recently attracted much attention due to their unique compositions, microstructures, and flexible properties. These alloys consist of multiple principle elements, and thus, a variety of different defects can be created in the material. Defects play a significant role on defining the material properties, in particular the mechanical properties. However, its role is far from being understood. Positron annihilation spectroscopy (PAS) is used to study the defects in CoCrFeMnNi.

The positron lifetime measurements performed on this alloy showed an average positron lifetime of 156 ps, which is much higher than the bulk lifetime value (≈ 110 ps), indicating the existence of a high defect concentration in the alloy. The temperature-dependent positron lifetime measurements showed the presence of shallow positron traps. A defect-related lifetime of 220 ps is obtained at room temperature, which corresponds to most likely divacancy defect. The theoretical calculations for the defects in this alloy and coincidence Doppler broadening spectroscopy (CDBS) measurements are in progress in order to identify the microstructure of the observed defects.

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

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

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

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

Positron Spectroscopy of Intermetallic Hydrogen Storage Alloys Synthesis Based on Ti-Cr with C14 and C36 Laves Phases

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The possibility of obtaining hydrogen storage materials based on TiCr₂ intermetallic compounds by melting in glow discharge plasma and electron beam melting is shown. Applying the glow discharge plasma method leads to the formation of the Laves phase with a C36 structural type, while electron beam melting allow to obtain the Laves phase with C14 type It has been established that the formation of Laves phases with different structural types is associated with different cooling rates, which is related to the synthesis methods peculiarities of intermetallic compounds.

Positron spectroscopy carries out by means of positron lifetime spectroscopy (PLS) and Coincidence Doppler broadening spectroscopy (DBS). To clarify the positrons lifetime for the C36 and C14 phases, theoretical calculations were performed in the framework of the density functional theory in the software package Abinit.

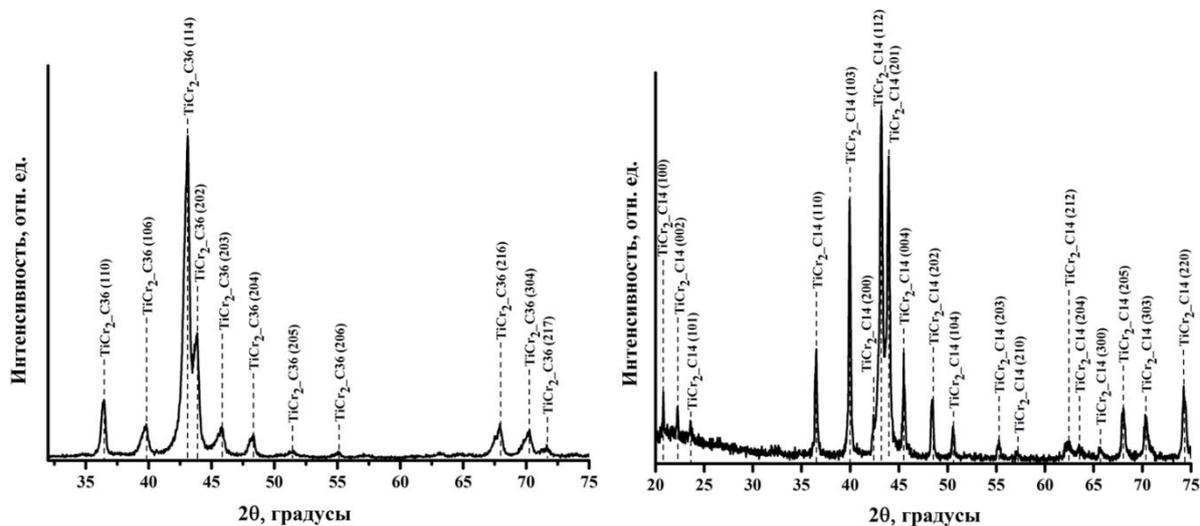


Fig1. Diffractograms of TiCr₂ alloys obtained in an anomalous glow discharge plasma (a) and electron-beam melting (b)

The research is carried out at Tomsk Polytechnic University within the framework of Tomsk Polytechnic University Competitiveness Enhancement Program grant.

Positron Spectroscopy of Defect Structure Additively Manufactured Titanium Ti-6Al-4V

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Nowadays additive manufacturing (AM) is being actively implemented in many industries. Among the advantages of AM in metals are the possibility of creating unique product shapes, providing solid and lightweight (e.g. lattice) structures in a single manufacturing process and high quality of resulting materials. Additionally, electron beam manufacturing (EBM) technology today provides high rates of production and layer-to-layer component quality control. . The use of additive manufacturing also allows creating a new generation of materials with unique set of properties. The same time few issues related to the EBM process in already well established AM materials like Ti and Ti-6Al-4V remain not clear. Present paper reports results of the first studies into the hydrogen interaction with titanium Ti-6Al-4V parts produced by EBM.

The research is funded from Russian Science Foundation (RSF), Grant Number №17-79-20100.

Improvement of depth resolution of VEPAS by simultaneous sputtering technique

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The poster shows a new method to improve the depth resolution by using Ar⁺ ions to remove the surface during the measurement of the Doppler-Broadening with monoenergetic positrons. The depth resolution becomes worst with higher positron energies because of the broadening of their implantation profile. To improve the depth resolution, the sample surface is removed by sputtering with argon ions during the DB measurement.

We could show that with this sputtering technique, it is possible to investigate layer systems of different materials and make the interfaces sharply visible. Furthermore, by using this method the investigation of whole solar cells and their defect structure is possible. Finally, the identification of a depth dependent defect profile inside an implanted Si sample was demonstrated.

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