ICPA-17 Summary Talks

R. Krause-Rehberg / Jerry Jean

- List will be not complete – We will be selective
- Only talks...
- I was in A sessions / Jerry in B sessions. Thus, we missed some important talk for our topics...
ICPA conferences

1965 ICPA  Detroit, USA
1971 ICPA-2 Kingston, Canada
1973 ICPA-3 Otaniemi, Finland
1976 ICPA-4 Helsingor, Denmark
1979 ICPA-5 Lake Yamanaka, Japan
1982 ICPA-6 Arlington, USA
1985 ICPA-7 New Delhi, India
1988 ICPA-8 Gent, Belgium
1991 ICPA-9 Szombathely, Hungary
1994 ICPA-10 Beijing, PR China
1997 ICPA-11 Kansas City, USA
2000 ICPA-12 Munich, Germany
2003 ICPA-13 Kyoto, Japan
2006 ICPA-14 Hamilton, Canada
2009 ICPA-15 Kolkata, India
2012 ICPA-16 Bristol, UK
2015 ICPA-17 Wuhan, China

50 years
187 participants from 23 countries:
- **89 China**
- 2 Argentina
- 2 Australia
- 2 Belgium
- 2 Canada
- 5 Czech Republic
- 2 Egypt
- 2 Finland
- 4 France
- **13 Germany**
- 1 Hong Kong
- 7 Italy
- **28 Japan**
- 6 Poland
- 1 Romania
- 3 Russia
- 2 Slovakia
- 1 Spain
- 2 Switzerland
- 1 Taiwan
- 2 Netherlands
- 4 UK
- 6 USA

- 4 plenary talks
- 39 invited talks
- 60 oral presentations
- 91 posters

= **194 contributions**
Some statistics (in red ICPA-17):
- ≈ 200 Participants (187)
- 160 contributing participants (194)
- 96 talks (103)
- among them 37 invited talks (43)
- 72 Posters (91)
- Contributions from 29 countries (23)
# Fields of Contributions

<table>
<thead>
<tr>
<th>Topic</th>
<th>Number</th>
<th>%</th>
<th>Who?</th>
</tr>
</thead>
<tbody>
<tr>
<td>Instrumentation</td>
<td>23 (22)</td>
<td>14 %</td>
<td>JJ</td>
</tr>
<tr>
<td>Semiconductors</td>
<td>7 (8)</td>
<td>5 %</td>
<td>RKR</td>
</tr>
<tr>
<td>Oxides / Ceramics</td>
<td>26</td>
<td>18 %</td>
<td>RKR</td>
</tr>
<tr>
<td>Metals / Alloys / Spin Polarized Positrons</td>
<td>37 (16)</td>
<td>20 %</td>
<td>RKR</td>
</tr>
<tr>
<td>Polymers</td>
<td>24 (10)</td>
<td>15 %</td>
<td>JJ</td>
</tr>
<tr>
<td>Mesopores</td>
<td>8</td>
<td>10 %</td>
<td>JJ</td>
</tr>
<tr>
<td>Membranes</td>
<td>15 (8)</td>
<td>10 %</td>
<td>JJ</td>
</tr>
<tr>
<td>General Theory (incl. Anti-Hydrogen)</td>
<td>12 (8)</td>
<td>8 %</td>
<td>RKR</td>
</tr>
<tr>
<td>Gases / Liquids</td>
<td>9</td>
<td>5 %</td>
<td>JJ</td>
</tr>
<tr>
<td>Other materials</td>
<td>5</td>
<td>3 %</td>
<td>RKR / JJ</td>
</tr>
</tbody>
</table>

JJ = Jerry Jean / RKR = Reinhard Krause-Rehberg
(numbers) = ICPA-16
- Instrument, 23
- Semiconductor, 7
- Oxides, 26
- Metals/Alloys, 37
- Polymers, 24
- Mesopores, 8
- Membranes, 15
- Fundamental theory, 12
- Liquids/Gases, 7
- Others, 3
• Many studies of Fe and steel, often for Fission / Fusion purposes
  – Not a simple material, but important field
  – 1V, 2V and dislocation lifetime is very similar
  – Precipitation, voids, grains and impurities in addition
  – ODS steel shows saturated e\(^+\) trapping without treatment
  – not more than 3…5 dpa (otherwise many gas-filled voids – nothing to see any more)
• W for Fusion: irradiation studies - much easier interpretation; e\(^+\) are very useful tool
• Al alloys: only a few studies – Positrons can still do a lot in this field (e.g. early stages of precipitation Al-Cu and Al-Mg-Si; defects in precipitation; role of vacancies)
• Combination with other methods: atom probe
• H in metals (steel, Ti)
• Very promising: Corrosion studies
• Spin-polarized positrons: important for spintronics; could be very surface sensitive (TOF); use of \(^{68}\text{Ge}\) allows higher polarization (70%); subjects: Ni; Heusler alloy;
• project of polarized beam: ELI-NP (Extreme Light Infrastructure) near Bucharest
• Nice study on high purity Ni(100) foils incl. XPS
• Ultra-fine grained steel
• Layers: W/Cu
Small but constant number of studies

- Very nice overview by Filip
- Defects in GaN for power devices
- Defects ion ZnO
- Photovoltaic research: CIGS layers
- PbSe and CdSe quantum dots
- Sulfur-hyperdoped Si
Perovskites is an important material class: vacancy identification by combination of PALS, CDBS and theory; dopant-induced vacancies; number of defects may be very large up to 1%

Question: positive vacancies might be visible when positive repelling potentials overlap each other? Oxygen vacancies are positive. But may be too small anyway?

UO₂ defect studies

Thermoelectric materials

Defects in SnO₂ films produced by sol-gel process

Ca-doping of BiFeO₃ ceramics

Effect of source irradiation: α-Al₂O₃ alumina at 10K long lifetime component changes

Sintering mechanism in fine-grained Silica
• Parameter-free gradient corrections for e+ states in oxides
• High-accuracy positron lifetime calculation
• First-principle calculations of e+ and Ps states near Bi₂TE₂Se
• Vacancy identification in ZnO, In₂O₃, and SnO₂
• Positron lifetime spectra evaluation by particle swarm optimization
• Positron diffusion in strong magnetic fields
• Positron scattering and annihilation on atoms and molecules

• Total-reflection high-energy Positron Diffraction (TRHEPD): determination of surface structure at outmost layer of surface; can clarify old puzzles of surface science -> very promising new positron technique
• Anti-Hydrogen research is continued: GBAR; ALPHA, AEgIS: resonant transitions observed between hyperfine states
• X- and Y-cut of natural quartz: stereoisomer behavior? More date required
• Study of native defects in topological insulator Bi₂Se₃ -> very hot topic
Marco John: Improvement of Depth resolution by Sputtering the sample

- Investigation of the whole solar cell, especially near the back contact
- In-situ sputtering
  - No air contact between the measurements
  - No degradation on the surface
  - Shorter overall measurement time

Sputter parameters: $I_B = 6 \text{ mA}; U_B = 400 \text{ V}$
<table>
<thead>
<tr>
<th>#Papers</th>
<th>Topic/Materials</th>
<th>(paper%)</th>
<th>Rank</th>
<th>Sum Talks</th>
</tr>
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<tbody>
<tr>
<td>37</td>
<td>Metals/Alloys</td>
<td>23</td>
<td>1</td>
<td>RK</td>
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<td>4</td>
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<tr>
<td>7</td>
<td>Liquids/Gases</td>
<td>4</td>
<td>8</td>
<td>JJ</td>
</tr>
<tr>
<td>3</td>
<td>Others</td>
<td>2</td>
<td>10</td>
<td>RK/JJ</td>
</tr>
<tr>
<td>162</td>
<td>Total # papers</td>
<td>100%</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Total: 162 papers
Instrumentation

- Surko’s trap: 7 meV cryogenically cooled gas
- NEPOMUC: Low-energy High-Intensity $10^9 e^+/s$
- New positron beams: McMaster, UTA, ELI-NP, ...
- TRHEPD Total-Reflection High-Energy Positron Diffraction
- Spin polarized positron beams
- Other techniques: PET, SEM, TEM, AFM, GPC, BET, XRD, SAXS, FTIR, EP, SIMS, UV-vis; LEED, XPS, ...
Fukaya: Development of LINAC-based TRHEPD (2010~)


Intensity is \(~100\) times larger than RI beam

\[5 \times 10^7\ e^+/sec\]

\[\sim 5 \times 10^5\ e^+/sec\]

Energy-tunable (< 35 keV)

Linear accelerator (LINAC)

Converter/moderator

Slow Positron Facility, KEK
Structure of graphene/Co(0001)

Optimum atomic positions

\[ \Delta = 0.01 \text{ Å} \pm 0.04 \text{ Å} \]

\[ \Delta_z = -0.15 \text{ Å} \pm 0.02 \text{ Å} \]

Rocking curves for graphene on Co(0001) substrate (one-beam condition)

\[ d = 2.06 \text{ Å} \pm 0.04 \text{ Å} \]

\[ d \text{ (Gr/Co)} \ll d \text{ (graphite)} \]

(Graphene on Co(0001) has no buckled structure)

Strong interaction with substrate

Y. Fukaya et al., in submission.
Polymers, Organic macromolecules

- Sub-nanometer free-volume size, fraction
- Free-volume theory and Ps-free volume
- Phase transitions
- Crystallinity and interfaces
- Molecular designs for devices
- Drug/nutrient transport
- Radiation effects
Chemical structures of TTPI(A), FPTTPI(B) and 2(FP)TTPI(C)
Results and Discussions

Dielectric properties of the PI films and a DuPont™ Kapton® polyimide film.

$k$ value at 10 kHz:
- Kapton film: 3.49
- TTPI: 1.68 (3.10 Å)
- FPTTPPI: 1.52 (3.24 Å)
- 2(FP)TTPI: 1.66 (3.07 Å)
Alam, A.: Edible biopolymer + sucrose + processing biopolymer + bioactive + water

- Expected trends in hole volume with varying water content as in model systems
- Expected trends in $T_g$
- Expected trends in hole vol. dispersion with water activity

Complex but still manageable carbohydrate matrices for comparison
Membranes

- Gas transport diffusivity, permittivity, and selectivity and free-volume
- Free-volume size control transport phenomena
- Asymmetric membranes – multi-layers
- Crystallinity and interfaces
- Desalination
- Molecular designs for devices
Sun, Y.M.: Structure Behaviors of Isothermally Annealed Isotactic Poly(4-methyl-1-pentene) Membranes Characterized by Positron Annihilation Lifetime Spectroscopy
Kinetic Molecular Diameter

$O_2$ 3.46 Å

$N_2$ 3.64 Å

$\tau_{3a}$ and $I_{3a}$ increase → Selectivity↑

$\tau_{3b}$ and $I_{3b}$ increase → Permeability↑

Free volume radiu (Å)

PDF

Lifetime (ns)

Permeability (barrer)

Crystallinity (%)
Proposed Model of gas transport through \( i \)-PMP

Three-phase model

Isothermal recrystallization
Mesopores

- Ps yield/production
- Theoretical models: quantum vs classical
- Inner surface chemical modification
- Pore filling
- Molecular designs for devices
He, C.Q: surface modification of inner surfaces

Trimethylsilylation @ \( \sim 100^\circ C \) for 3 hours

\[-\text{OH} + (\text{CH}_3)_3\equiv\text{Si-Cl} \rightarrow -\text{O-Si} \equiv(\text{CH}_3)_3 + \text{HCl}\]

1. Pore architecture is unchanged;
2. Pore size becomes smaller.
Ps lifetime and pore surface chemistry

Ps-surface interaction depends on surface chemistry. *(C. He et al., PRB 75, 195404 (2007))*;

Note: pore size decreases by 0.5 nm (N₂ adsorption)! Inconsistent?
Positron lifetimes were measured with different relative humidities.
RH dependence of o-Ps lifetime and intensity for different components.

Subnanohole size of 2nd comp. reduces with increased RH due to water adsorption, while the smaller hole size of 1st comp. is independent on RH.
Gases/Liquids

- Positron-atomic scattering
- Scattering theories
- Ps formation in liquids
- Ps-bubble in liquids
Others

- Zhang, R. : Study of Defects in Ferroelectric Croconic Acid Single Crystals
- J.David van Horn: chiral molecules, quartz, tartaric acids
- Zhong, J.: Graphene, and graphene oxides
- Shi, W. : Colloidal quantum dots
- Zgardoynska: Encapsuled nano polymer/alkane
Two Personal Encouragements

• Cultivate young generations to positron science
• Cooperation and collaborations *inter and intra*

Thank ICPA17 excellency,
Welcome to USA for ICPA18
God Bless You