Selecting the Right icpTOF for Your Research

TOFWERK Webinar, Martin Tanner
• Why TOFMS for inorganic analyses
• Important aspects of inorganic analyses
• icpTOF models and performance
TOF Principle

Why TOFMS

Measured Time Dependent Signal

Detector
T-Flight depends on m/q

TOF-Extraction
Acceleration to equal E

Primary Ion Beam

Reflector

Mass Calibration

202 204 206 208 210
m/q [Th]
The major advantages of TOFMS

• Always full mass spectra
• Large number of analytes in milliseconds => TOFMS
• Example:
  • micro droplet generator sampling
  • 500 ppb multi-element solution
  • 40 µm droplets
  • <1 ms signal per droplet
  • 30 µs time resolution
Single Particles & Cells

Quantification
- Better S/N by dilution
- Mass and #-conc.

Analyte mass per particle

Particle number conc.

Single Particles & Cells

**Distinction by Composition**

- Mixture of 50 nm Au NPs and 60 nm AgAu coreshells
- 36 µs time resolution (trigger mode)
- Temporal separation of pure Au NPs and coreshell NPs.
- Single events ~0.5 ms.
Fast Laser Ablation

Basic principles of laser ablation

• Ablation of material
• Aerosol transport
• Ionisation in ICP
• Measurement of sampled ions
• Fast washout allows resolution of individual laser pulses

• Example:
  • Laser: Teledyne CETAC, Analyte G2 with Cobalt cell
  • Sample: SRM NIST612
  • 10 µm spot size, 300 Hz
Fast Laser Ablation

**Information through Image**
- Mineral Formation
- Alterations (Metamorphoses)

**Example: Mineral Mapping**
- Sample: Micashist garnet
- Courtesy of Gavril Săbău, Geological Institute of Romania
- Laser: Teledyne CETAC Analyte G2 + Cobalt cell
- 5 µm spot size, 150 Hz
- 410 kpixel, acquired in ~2 h
- Data processing in HDIP (Teledyne)
• Why TOFMS for inorganic analyses
• **Important aspects of inorganic analyses**
• icpTOF models and performance
Signal Dynamics

Full Mass Range & Full Signal Range

- Get used to Log scale!
- TOFMS baseline affected by intense signals
- Baseline must be measured for postprocessing
- Baseline should be continuous for accurate subtraction
Interference Control

**Qcell**

- Collisions for ion cooling: improving mass resolution and sensitivity
- Reactions: interference control
- Example: Reaction with H₂
  - Elimination of polyatomic interferences
  - Detection of Fe, K, Ca significantly improved
Attenuation of matrix ion current

• Less ions in TOF extraction
• Lower MS baseline
• Avoid detector saturation
• Example: LA of Zircon
  • Attenuation for Zr and Hf
  • Less stray ions.
  • Improved U/Pb dating
Full Mass Spectra

Particles and Cells

- No analytes get ‘forgotten’
- Simultaneous detection of particles and ionic background

**Application Aspects**

<table>
<thead>
<tr>
<th>NPs</th>
<th>Signal (counts)</th>
</tr>
</thead>
<tbody>
<tr>
<td>50 nm Au</td>
<td>225</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Ions in Solution</th>
<th>Sensitivity (cps/ppb)</th>
</tr>
</thead>
<tbody>
<tr>
<td>59Co</td>
<td>5.2e4</td>
</tr>
<tr>
<td>115In</td>
<td>1.25e5</td>
</tr>
<tr>
<td>197Au</td>
<td>6.3e4</td>
</tr>
<tr>
<td>238U</td>
<td>3.5e5</td>
</tr>
</tbody>
</table>
Data Postprocessing

- Time dependent mass calibration
- Deconvolution of analyte peaks and interferences
- (Low mass) ions as internal standard for LA quantification
- Baseline correction for accurate trace element quantification
• Why TOFMS for inorganic analyses
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Instrument Layout

**TOFWERK**
- Notch filter
- TOFMS

**Thermo iCAP RQ**
- ICP source
- Water cooled interface
- Primary ion optics
- Qcell
- >1000 units installed per year worldwide

**icpTOF**
Pairing leadership in ICP and TOFMS!
TOFMS - Versions

icpTOF R
- Res 3000
- Most Versatile
- Single Particles
- Geochemistry

icpTOF 2R
- Res 6000
- Best Accuracy
- Geochemistry
- Geochronology
- Nuclear Forensics
- Phosphorus & Sulphur

icpTOF S2
- Highest sensitivity
- Single Particles/Cells
- Bio-Imaging
Linear Response

icpTOF S2, R, 2R

- ‘Linearity’ – a must-have for quantitative Analyses
- All icpTOF versions provide >6 orders of magnitude linear response

**238U Sensitivity**
Liquid sample introduction by standard nebulizer and spray chamber

**197Au Sensitivity in particles**
icpTOF S2: sub fg quantitative measurement

![Graph showing linear response and sensitivity](image)

- R-squared: 0.999
- Concentration (ppb) vs. Signal intensity (cps)
- Data, Fit, Confidence bounds

**Sensitivities**
- 20
- 50
- 71
- 80
- 89
IcpTOF - Versions

**icpTOF S2**
- Highest sensitivity: 300'000 cps/ppb (\(^{238}\)U)
- Unit mass resolution
- Best for signal limited applications (ultra short signals)

**icpTOF R**
- Sensitivity: 50’000 cps/ppb (\(^{238}\)U)
- MS resolution: 3’000 Th/Th
- Broad range of applications (particles, imaging, geochemistry)

**icpTOF 2R**
- Sensitivity: 30’000 cps/ppb (\(^{238}\)U)
- Highest MS Resolution: 6’000 Th/Th
- Best background limited applications (trace elements and isotope ratios)
Sensitivity - Single Particles

icpTOF S2

- Highest sensitivity for single particles
- Example: 20 nm Gold particles
- Time resolution: 0.1 ms
- Background: $<< 1$ count per integration time
- S/N cannot be improved by lowering background but only by increasing signal intensity
- Sensitivity limited application!

20 nm Au Particles
Time dependent signal: 0.1 ms resolution

![Signal vs Time Graph](image)
Sensitivity - Single Cell LA Imaging

**icpTOF S2**
- Highest sensitivity for small laser spot size
- Natural element concentrations in individual muscle cells
- ESL NWRimage 266nm laser
- 1 µm spot size
- Sample courtesy: Amy Managh, Loughborough University
Unbiased Signal Range

icpTOF 2R

- < 1 ppm to >10’000 ppm quantitative LA data from µm-size spots
- Laser: Analyte G2, Teledyne CETAC
- Spot size: 5 µm, Frequency: 100 Hz
- Sample: Garnet from a metamorphic rock
- Courtesy of Tom Raimondo, Adelaide
- Image Size: 600x650 pixel
- Acquisition time: 5h45m
- Reference material: NIST610
- Internal Standard: $^{28}$Si
Accurate Ratios

**icpTOF R: Accurate element ratios for U/Pb dating**
- Accurate ratios
- $^{206}\text{Pb}/^{238}\text{U}$ ratio $<1\%$

**icpTOF 2R: Accurate isotope ratios for nuclear forensics**
- Precision and accuracy improved for increased number of integrated $^{235}\text{U}$ counts (as expected)
- $^{235}\text{U}/^{238}\text{U}$ ratios in good agreement with the reference IRs even of the lowest numbers of integrated counts
TOFpilot – Workflows

Particles Analyses

• Supporting all standard liquid analysis

• Particles/cells analyses and data evaluation

• Reports as PDF and CSV export
LA Imaging

- Reads geometry information from laser software
- Starts acquisition and fill data in pixel-by-pixel
- Pixel by pixel data acquisition triggering
- Live preview
icpTOF References

TOFMS experts since 2002

17 icpTOF units installed since 2013

>40 Peer reviewed publications on icpTOF data

1. Japan Automobile Research Institute (JARI), Japan, 2013
2. ETH Zurich, Switzerland, 2015
3. University of Tasmania (UTAS), Australia, 2016
4. Swiss Gemmological Institute (SSEF), Basel, Switzerland, 2016
5. University Vienna, Austria, 2017
6. University Bern, Climate and Environmental Physics, Switzerland, 2017
7. LGC Limited, Inorganic Analysis, UK, 2018
8. Academia Sinica AS-BCST, Taiwan, 2018
9. Universite du Quebec a Chicoutimi, Canada, 2018
10. Carnegie Mellon University CMU Pittsburgh, USA, 2018
11. Ghent University, Belgium, 2019
12. University of South Carolina, Columbia, USA, 2020
13. BAM Berlin, Germany, 2019
14. UFZ Leipzig, Germany, 2019
15. Iowa State University, Ames, USA, 2020
16. KRISS Daejeon, Korea, 2019
17. University of Tokyo and Nuclear Regulation Authority, Japan, 2019
Smallest Footprint

icpTOF S2 and icpTOF R

icpTOF 2R
Installed Systems

icpTOF 2R

icpTOF R with Laser
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