

MS 9: New Developments II

Time: Friday 10:45–12:00

Location: H2

Invited Talk

MS 9.1 Fri 10:45 H2

Spatially resolved ultra-trace analysis of actinides on hot particles by resonant laser-SNMS — ●HAUKE BOSCO¹, MARTIN WEISS¹, MANUEL RAIWA¹, NINA KNEIP², KLAUS WENDT², and CLEMENS WALTHER¹ — ¹Institute of Radioecology and Radiation Protection, Leibniz University Hannover — ²Institute of Physics, Johannes Gutenberg-University Mainz

A titanium:sapphire resonance excitation laser system for element selective ionization of sputtered neutrals has been linked to a commercial TOF-SIMS for spatially resolved ultra-trace isotope detection [1]. The system allows analysis of stable and radioactive isotope ratios with 70 nm spatial resolution. Synthetic as well as environmental samples are measured on either conducting or non-conducting samples. As an example, investigations of hot particles from the Chernobyl exclusion zone will be presented and discussed with respect to isotopic ratios of uranium, plutonium, americium and strontium. By suppression of isobaric interferences minor actinide isotopes on the scale of a few fg were detected within the analyzed fuel matrix. Additionally, Pu-238 was unambiguously identified despite five orders of magnitude of U-238 isobaric contamination. Ongoing excitation scheme development, influences of the plutonium hyperfine structure on the resulting isotope signal and single particle analysis will be presented as a part of the BMBF funded project SIRIUS.

[1] Franzmann et al., Resonant laser-SNMS for spatially resolved and element selective ultra-trace analysis of radionuclides, JAAS 2018

Invited Talk

MS 9.2 Fri 11:15 H2

Multi-reflection time-of-flight mass spectrometry for cluster research — ●PAUL FISCHER and LUTZ SCHWEIKHARD — Institut für Physik, Universität Greifswald, 17487 Greifswald, Germany

Multi-reflection time-of-flight mass spectrometry (MR-ToF MS) is known as a powerful tool for precision mass measurements [1] and high-resolution isobar separation [2] in nuclear physics. In atomic and molecular physics, MR-ToF devices are appreciated for their characteristics as electrostatic ion traps [3]. However, they are often operated in non-bunching mode, abandoning high resolving powers in favor of easier interaction prerequisites.

At the University of Greifswald, MR-ToF MS is applied for high-

resolution investigations of atomic clusters. Techniques for in-trap photodissociation, tandem MR-ToF MS, and the study of time-delayed dissociation processes have been developed. Examples include the dissociation behavior of bismuth clusters [4], the change thereof resulting from doping with a single lead atom [5], and the delayed dissociation of indium clusters [6].

[1] F. Wienholtz et al., Nature 498:346-349 (2013)

[2] R.N. Wolf et al., Phys. Rev. Lett. 110:041101 (2013)

[3] D. Zajfman et al., Phys. Rev. A 55:R1577-R1580 (1997)

[4] P. Fischer et al., Eur. Phys. J. D 73:105 (2019)

[5] P. Fischer et al., Phys. Rev. Research 1:033050 (2019)

[6] P. Fischer et al., Phys. Rev. Research 2:043177 (2020)

MS 9.3 Fri 11:45 H2

Development of a Python application for isotope pattern analysis of small metal complexes measured with an Orbitrap analyzer and electrospray ionization — ●ANNA KOGIOMTZIDIS, JULIA STADLER, MICHAEL STEPPERT, and CLEMENS WALTHER — Institute of Radioecology and Radiation Protection, Leibniz University Hannover, Germany

Isotope pattern analysis is a well established method for the evaluation of mass spectral data. Especially in metabolomics and proteomics it is widely used. While these research fields concentrate mainly on relatively large biomolecules, this work focuses on metal ions complexed by anorganic or small organic ligands. This type of compound is relevant for instance in the context of radioecology when studying the transport behavior of radionuclides in different chemical environments.

A Python module plus graphical interface was developed to assist with the investigation of metal complexes by mass spectrometry. The application includes two main functionalities. First, an algorithm was implemented to scan mass spectra for peak groups matching a given isotope pattern in order to identify compounds possibly containing an element of interest. Second, it is possible to search for specific chemical species defined by molecular formulas. Further, some additional features including data preprocessing and calculation of possible sum formulas for a given signal are available.

The software was tested with several solutions of europium, zirconium and uranium with natural isotope abundances to examine a range of different isotopic configurations.