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Characterization of nanoparticles in food using ICP-MC - how far have we come in the last 10 years?

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9th Nordic Conference on Plasma Spectrochemistry

June 10 - 13, 2018
Loen, Norway

Programme and Abstracts

1   Table of Content

2   Welcome Letter

Dear colleagues,
On behalf of the Analytical Section of the Norwegian Chemical Society and the Organising Committee it is an honour and pleasure to welcome you to Loen and the 2018 Nordic Conference on Plasma Spectrochemistry. This conference provides both an international and regional forum by which researchers and users have the opportunity to share their knowledge and exchange ideas.

The plenary programme has been planned with a view of furnishing a comprehensive overview of the latest developments in this scientific field. Since some of the world's leading authorities will be present, the conference will hopefully be a stimulating forum for communication across borders and between scientific disciplines.

In contrast to other plasma spectrochemistry meetings, short tutorial courses will be offered to all participants during the three-and-a-half-day meeting which may be attractive to participants who can learn about or to be updated on plasma spectrochemistry and application. This concept is meant to stimulate especially Nordic users of plasma based techniques to learn more about theoretical and practical issues as well as to obtain specialists recommendations for method improvements.

We know that the natural beauty of the area will captivate you, but we also hope that the conference excursions, social events and outdoor farewell dinner may complement the scientific endeavours. We promise you an exciting and memorable conference and stay in Loen!

On behalf of the Organising Committee

Yngvar Thomassen
Chairman

3   Organising and Scientific Committee

Yngvar Thomassen (Chairman), National Institute of Occupational Health, Oslo and Norwegian University of Life Sciences, Ås, Norway
Balazs Berlinger, National Institute of Occupational Health, Oslo, Norway
Ivar Martinsen, GE Healthcare, Oslo, Norway
Arne Åsheim, (Exhibition coordinator), Molab AS, Porsgrunn Branch, Norway
Oddvar Røyseth, (Treasurer) Norwegian University of Life Sciences, Ås, Norway
Elin Gjengedal, Norwegian University of Life Sciences, Ås, Norway
Jens Sloth, Technical University of Denmark, National Food Institute, Denmark
Ari Väisänen, University of Jyväskylä, Finland
Walter Lund, University of Oslo, Norway

4   General Information

Conference Desk

The conference desk is situated in the conference foyer of Hotel Alexandra. It will operate as follows:

Saturday	June 9	16:00 - 18:00
Sunday	June 10	07:30 - 08:15
Monday	June 11	07:30 - 08:00
Tuesday	June 12	07:30 - 08:00
Wednesday	June 13	08:30 - 09:00

Participants are requested to register as soon as possible upon arrival to Hotel Alexandra, Loen.

Conference Venue

All oral and poster sessions will be held in the various auditoriums of Hotel Alexandra.

Tel: +47 57 87 50 00   Fax: +47 57 87 50 51   Email: alex@alexandra.no
Homepage: www.alexandra.no

Meals

Participants staying at Hotel Alexandra are served breakfast, lunch and dinner (all included in their accommodation package).

5   Social Programme

Saturday, June 9, 17:00 - 19:00 Informal get-together in the Hotel Alexandra Bath & Spa

All delegates and accompanying persons are invited to enjoy the heated outdoor swimming pool and refreshments. *This event is kindly sponsored by Holger Hartmann AS and Perkin Elmer.*

Sunday, June 10, 14:00: Half-day excursion to Geiranger

This tour encompasses a mountain plateau above the tree and snow lines, the summit of Dalsnibba (1746 m), and a sail of 25 km along the spectacular Geirangerfjord.
Price per person: NOK 700 (not included in the registration fee).

Sunday, June 10, 14:15: Guided walk to Bødal Glacier

On the Bødal Glacier in Loen Valley you can enjoy a genuine walking experience in beautiful West Norwegian surroundings. The whole trip, rated a moderately difficult hike, takes from five to six hours.
The Bødal Valley, with the Bødalseter summer pasture farms and the Bødal Glacier, is one of the gems of the Jostedalsbreen National Park. Take a rucksack, clothes, food and drink for a half day walk. Good strong mountain boots will be an advantage.

Free of charge.

Sunday, June 10, 14:15: Mountain hiking for fit spectroscopists: The Skåla Challenge

Those who want to challenge the Norwegian mountains are offered a guided walk after lunch to the Klaumann Tower at Skåla Mountain. This is the hardest uphill in entire Norway, approx. 1800 m straight up. Presently there may still be much snow above 1000 meters. Hikers are advised to bring appropriate footwear and clothing for this walk. Free of charge, but we promise; you will sweat!

Sunday, June 10, 14:15: Loen Skylift

Loen Skylift is a spectacular new attraction and adventure arena, at the inner part of the Nordfjord, in the heart of Fjord Norway. A Cable Car will lift you from the fjord to 1011 m. Here you can enjoy the views of the fjord landscape - from the restaurant table, or while exploring in the mountains. NOK 505 (not included in the registration fee).

Monday, June 11, 21:30: Bring your own wine

The cork fee charged by the hotel in order to bring own wine is kindly sponsored by Agilent Technologies and Matriks AS.

Tuesday, June 12, 16:30 Excursion to the Briksdal Glacier with a conference outdoor dinner

You are invited to visit the heart of Norway - an **Unforgettable** trip to the Briksdal Glacier. Participants can enjoy a walk to view the enormous cascade of ice where you will be able to test the best aquavit in the world; *Gilde Aqua Ultra Plus*, *sponsored by Agilent Technologies and Matriks AS.*

Afterwards there will be the famous outdoor barbeque at "Kleivane" (weather permitting - otherwise the grill party will be held at Briksdalen Inn).
The well-known Norwegian gourmet chef Frode Aga will once again be in charge of the kitchen to ensure your best outdoor food experience.
This event is kindly sponsored by Cameca - Nu, Thermo Fisher Scientific and Shimadzu Europa.

6   Scientific Programme

Oral presentations
Invited plenary lectures and submitted oral contributions will be 25 and 15 minutes in length, respectively (including discussion).
Video projectors will be provided in all lecture rooms.

Posters
The posters should be mounted during Saturday evening, June 9 and in the early morning on Sunday June 10, in the poster area located next to the lecture room. Materials for poster mounting are available either from the conference desk or in the poster mounting area.

Language
The working language of the conference is English.

7   Liability

The Organising Committee declines any responsibility whatsoever for injuries or damages to persons or their property during the conference.

8   Sponsors and exhibitors

The conference is sponsored by:

The exhibition of scientific instrumentation, literature and consumables is located next to the auditorium in the first floor.

The following companies have registered for display and demonstration:

> Element Scientific Inc.
> Holger Hartmann AS / PerkinElmer
> Houm
> Matriks AS / Agilent Technologies
> Cameca / Nu Instruments
> Shimadzu Europa GmbH
> Thermo Fisher Scientific / NerliensMeszansky
> Teknolab
> Postnova / Nordlab

9   Correspondence after the conference

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E-mail: Yngvar.Thomassen@stami.no

10   Schedule of events

Saturday, June 9, 2018	
16:00 - 18:00	**Registration**
17:00 - 19:00	**Informal get-together in the Hotel Alexandra Bath & Spa** This event is kindly sponsored by Holger Hartmann AS and Perkin Elmer
19:00	**Dinner**

Sunday, June 10, 2018	
07:30 - 08:15	**Registration**
08:00 - 08:15	**Welcome and opening remarks**
08:15- 13:00	**Plenary session I: Progress in plasma spectrochemistry** **Poster viewing and exhibition**
13:00	**Lunch**
14:00 (14:15)	**Excursion to Geiranger, The Skåla Challenge,** **guided walk to Bødal Glacier and Loen Skylift**
19:00	**Dinner**

Monday, June 11, 2018	
08:00 - 11:55	**Plenary session II: Bio-imaging and speciation** **Poster viewing and exhibition**
11:55 – 13:00	**Plenary session III: Applications of plasma spectrochemistry** **Poster viewing and exhibition**
13:00 - 14:15	**Lunch**
14:15 – 15:40	**Plenary session III continues: Applications of plasma spectrochemistry** **Poster viewing and exhibition**

Monday, June 11, 2018 cont.			
Short course session 1			
15:55 - 17:40	**Short course A1**	**Short course A2**	**Short course A3**	**Short course A4**

17:40 - 17:55   **Coffee break, exhibition and poster viewing**

Short course session 2			
17:45 -19:40	**Short course B1**	**Short course B2**	**Short course B3**	**Short course B4**
19:40	**Dinner**			
21:30	**Poster viewing and discussions with wine tasting** **(Bring your own wine)** This event is sponsored by Matriks AS and Agilent Technologies			

Tuesday, June 12, 2018	
08:00 - 08:10	**The Nordic Plasma Torch Award**
08:10 – 11:10	**Plenary Session IV: Single particle and single cell analysis by plasma spectrochemistry** **Poster viewing and exhibition**
11:10 – 13:20	**Plenary Session V: New analytical capabilities**
13:20 - 14:20	**Lunch**
Short course session 3	
14:20 - 16:05	**Short course C1** **Short course C2** **Short course C3**
16:30	**Excursion to Briksdal Glacier and conference outdoor dinner** This event is kindly sponsored by Cameca - Nu, Thermo Fisher Scientific and Shimadzu Europe

Wednesday, June 13, 2018		
08:30 – 09:30	Plenary session VI: Radioisotopes and isotopic ration measurements		
	Short course session 4		
09:30 - 11:30	Short course D1	Short course D2	Short course D3
11:30 – 11:45	Closing remarks and farewell		
12:00	Lunch		

11   Daily Programme

Sunday, June 9, 2018

Time	Abstr.	
Time	**Abstr.**	
08:00-08:15		**Welcome/Opening remarks** Yngvar Thomassen, Conference chairman

Session I: Progress in plasma spectrochemistry

Chairman: Yngvar Thomassen

Distinguished Speakers' Lectures:

08:15-08:45	O-1	**Physics of technological ICP: Beginning of understanding** <u>Albert Gilmutdinov</u>, M. Voronov, K. Nagulin, I. Tsivilskiy Kazan National Research Technical University, Russia
08:45-09:15	O-2	**Plasma spectrochemistry and its relatives** <u>Gary M. Hieftje</u>[1], A. J. Schwartz[1], J. T. Shelley[2], Y. Cheung[1], K. M. Thaler[3], C. E. Cissna[1], G. C. Roesch[1] [1]Department of Chemistry, Indiana University, Bloomington, USA [2]Department of Chemistry, Rensselaer Polytechnic Institute, Troy, USA [3]Institute of Hydrochemistry, Technische Universität München, Germany
09:15-09:40	O-3	**Physics of spectroanalytical ICP: Finalization of understanding** <u>Ilya Tsivilskiy</u>, A. Gilmutdinov, B. Khamidullin, K. Nagulin Kazan National Research Technical University, Russia
09:40-10:05	O-4	**Particle transport in the ICP torch: What modeling reveals?** Maryam Aghaei, Department of Chemistry, University of Antwerp, Belgium
10:05-10:25		**Coffee, exhibition and poster viewing**

Session I continues: Progress in plasma spectrochemistry
Chairman: Jens J. Sloth

Time	Abstr.	
10.25-10:50	O-5	**Atmospheric-pressure plasmas as ionization sources for atomic, molecular, and biological mass spectrometry**

Jacob T. Shelley[1], S. P. Badal[1], C. L. Walton[1], A. J. Schwartz[2], G. M. MacLean[1], I. Ayodeji[3], G. C.-Y. Chan[4], J. Wu[1], M. Burnley[1], T. Evans-Nguyen[3]
[1]Department of Chemistry and Chemical Biology, Rensselaer Polytechnic Institute, Troy, USA, [2]Department of Chemistry, State University of New York at Buffalo, USA
[3]Department of Chemistry, University of South Florida, Tampa, USA
[4]Laser Technologies Group, Lawrence Berkeley National Laboratory, Berkeley, USA

| 10:50-11:15 | O-6 | **A new generation of solid-state detectors for mass spectrometry** |

Steven J. Ray,
University of Buffalo, USA

| 11:15-11:40 | O-7 | **Direct sampling and analysis of airborne particulate organic matter by proton-transfer-reaction mass spectrometry** |

P. Eichler[1], M. Müller[1,2], Armin Wisthaler[1,3]
[1]Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Austria,
[2]Ionicon Ionicon Analytik Ges.m.b.H., Innsbruck, Austria
[3]Department of Chemistry, University of Oslo, Norway

| 11:40-12:05 | O-8 | **Recent spectrochemical emerging advances and applications in environmental monitoring** |

Tero Eklin
Finnish Environmental Institute (SYKE), Helsinki, Finland

| 12:05-12:20 | O-9 | **Flowing atmospheric pressure afterglow for ionization in electrochemistry/mass spectrometry** |

Valerie A. Brückel, M. Sperling, U. Karst
Institute of Inorganic and Analytical Chemistry, University of Münster, Germany

| 12:20-12:45 | O-10 | **Quantitative bioimaging by LA-ICP-MS as a tool to support toxicological and medical investigations** |

Michael Sperling, S. Fingerhut, D. Dietrich, R. Buchholz, J.-C. Müller, U. Karst
Institute of Inorganic and Analytical Chemistry, University of Münster, Germany

| 12:45-13:00 | O-11 | **Visualizing elemental deposition patterns on graphite anodes from lithium ion batteries: A combination of laser ablation-inductively coupled plasma-mass spectrometry and laser ablation-inductively coupled plasma-optical emission spectrometry** |

Sascha Nowak[1], T. Schwieters[1], C. Lürenbaum[1], M. Mense[1], B. Vortmann-Westhoven[1], M. Winter[1,2]
[1]MEET Battery Research Center, Institute of Physical Chemistry, University of Münster, , Germany, [2]Forschungszentrum Jülich GmbH, Helmholtz-Institute Münster, Germany

13:00-14:15		**Lunch**
14:15		**Excursion to Geiranger, the Skåla challenge, guided walk to Bødal Glacier and Loen Skylift**
19:00		**Dinner**

Monday, June 11, 2018

Session II: Bio-imaging and speciation
Chairman: Jacob T. Shelley

Time	Abstr.	
08:00-08:25	O-12	**Elemental bioimaging and speciation analysis to track gadolinium from MRI contrast agents in the brain** Uwe Karst, University of Münster, Germany
08:25-08:50	O-13	**Completing the jigsaw: multi-modal approaches to investigate brain iron in health and disease** Joanna Collingwood, University of Warwick, United Kingdom
08:50-09:15	O-14	**Quantification of metalloproteins relevant to human health using complementary hyphenated techniques and isotope dilution ICP-MS** Heidi Goenaga-Infante, R. Larios, C. W. Dietrich, M. E. del Castillo Busto LGC Ltd, Teddington, United Kingdom
09:15-09:40	O-15	**Elemental labelling as a general platform for ICP-MS analysis of clinical biomarkers** Maria Montes-Bayón, F. J. Alonso García, E. Blanco-González Department of Physical and Analytical Chemistry, Faculty of Chemistry, University of Oviedo, Spain
09:40-10:05	O-16	**Quantitation of peptides by selenium labeling** L. H. Møller, F. Grønbæk-Thorsen, S. Stürup, Bente Gammelgaard Department of Pharmacy, University of Copenhagen, Denmark
10:05-10:25		**Coffee break, exhibition and poster viewing**
10:25-10:40	O-17	**Arsenic speciation analysis elucidates the risk assessment of food supplements with ingredients of marine origin** Karlien Cheyns, H. Demaegdt, N. Waegeneers, A. en Ruttens Sciensano, Tervuren, Belgium
10:40-10:55	O-18	**Survey of arsenic species in the top 10 most consumed seafoods in the US** Sean D. Conklin, M. M. Wolle Food and Drug Administration, College Park, USA
10:55-11:10	O-19	**Fast arsenic speciation analysis of wine, and rice by LC-ICP-QQQ** C. Tanabe[1], S. E. Ebeler[1], J. Nelson[1,2], Raquel Larios[3] [1]Department of Viticulture and Enology, University of California, Davis, USA [2]Agilent Technologies Inc., Santa Clara, USA [3]Agilent Technologies Inc., Madrid, Spain
11:10-11:25	O-20	**Selenium speciation in feed by HPLC-ICP-MS** Hanneke Brust, S. Frankhuizen, M. van der Lee RIKILT, Wageningen, The Netherlands

Session II continues: Bio-imaging and speciation
Chairman: Jacob T. Shelley

Time	Abstr.	
11:25-11:40	O-21	**A study of selenoproteins in atlantic salmon (*salmo salar*) using hyphenated mass spectrometry and bioinformatics**

Veronika Sele[1], M. Perez[2], A. Raab[2], M. Mariotti[3], E. Krupp[2], J. Feldmann[2], J. J. Sloth[4,1], R. Ørnsrud[1], M. H.G. Berntssen[1], J. D. Rasinger[1]
[1]Institute of Marine Research (IMR), Bergen, Norway
[2]TESLA, Department of Chemistry, University of Aberdeen, Scotland, UK
[3]Division of Genetics, Department of Medicine, Brigham and Women`s Hospital, Harvard Medical School, Boston, USA
[4]National Food Institute, Technical University of Denmark, Lyngby, Denmark

| 11:40-11:55 | O-22 | **Binding of ethylmercury from thiomersal to hemagglutinin in influenza vaccines** |

Philipp Strohmidel[1], M. Sperling[1,2], U. Karst[1]
[1]University of Münster, Germany, [2]EVISA, Münster, Germany

Session III: Applications of plasma spectrochemistry
Chairman: Joanna Irrgeher

| 12:00-12:15 | O-23 | **Purity determination of high purity metals – considerations from a metrology perspective** |

Panayot Petrov, D. N. Douglas, J. Entwisle, S. Hill, H. Goenaga-Infante
LGC Ltd, Teddington, United Kingdom

| 12:15-12:30 | O-24 | **Metallurgical analysis with ICP-OES: Dealing with the matrices and interferences** |

K. Neubaurer, Erica Cahoon
Discovery & Analytical Solutions, Perkin Elmer Inc., Shelton, United Kingdom

| 12:30-12:45 | O-25 | **Trace analysis of emerging contaminants in riverine, estuarine and coastal systems using ICP-MS/MS and hyphenated techniques** |

Daniel Pröfrock[1], J. Irrgeher[1], J. Meinke[1,3], T. Orth[1,4], A. Reese[1,2], T. Zimmermann[1,2]
[1]Centre for Materials and Coastal Research, Institute of Coastal Research, Department Marine Bioanalytical Chemistry, Helmholtz-Zentrum Geesthacht, Germany
[2]Department of Chemistry, Institute for Inorganic and Applied Chemistry, Universität Hamburg, Germany, [3]Department of Applied Natural Sciences, Fachhochschule Lübeck, University of Applied Science, Germany, [4]Hochschule Mannheim, Germany

| 12:45-13:00 | O-26 | **Quantitative metabolite profiling of medical drugs via high-performance liquid chromatography-inductively coupled plasma mass spectrometry after pre-column derivatization** |

Sanwang Li[1], B. Klencsár[1], L. Balcaen[1], F. Cuyckens[2], F. Lynen[3], F. Vanhaecke[1]
[1]Department of Analytical Chemistry, Ghent University, Belgium
[2]Pharmacokinetics, Dynamics & Metabolism, Janssen R&D, Beerse, Belgium
[3]Department of Organic and Macromolecular Chemistry, Ghent University, Belgium

| 13:00-14:15 | | **Lunch** |

Session III continues: Applications of plasma spectrochemistry
Chairman: Jörg Bettmer

Time	Abstr.	
14:15-14:40	O-27	**Determination of technologically critical elements in environmental and clinical samples by ICP-MS** Ilia Rodushkin[1,2], E. Engström[1,2], D. C. Baxter[2] [1]Division of Geosciences, Luleå University of Technology, Sweden [2]ALS Laboratory Group, ALS Scandinavia AB, Luleå, Sweden
14:40-14:55	O-28	**Iodine in seaweed - occurrence, speciation, bioavailability and risk assessment** Jens J. Sloth[1], A. Duinker[2], M. Hansen[1], S. Holdt[1] [1]National Food Institute (DTU Food), Technical University of Denmark, KGS Lyngby, Denmark, [2]Institute of Marine Research, Bergen, Norway
14:55-15:10	O-29	**Multimodal elemental and molecular imaging analysis of drugs on abuse on blotter papers** Michael Holtkamp[1], E. Lützen[1], I. Stamme[2], M. Pütz[2], M. Sperling[1],U. Karst[1] [1]Institute of Inorganic and Analytical Chemistry, University of Münster, Germany [2]Forensic Science Institute, Federal Criminal Police Office (BKA), Wiesbaden, Germany
15:10-15:25	O-30	**Identification and quantification of potentially hazardous decomposition products of lithium ion battery electrolytes chromatographic techniques with ICP-SF-MS detection** Yannick P. Stenzel[1], J. Henschel[1], M. Winter[1,2], S. Nowak[1] [1]MEET Battery Research Center, Institute of Physical Chemistry, University of Münster, Germany, [2]Forschungszentrum Jülich GmbH, Helmholtz-Institute Münster, Germany
15:25-15:40	O-31	**Investigation of lithium losses in lithium ion batteries by means of plasma based techniques using isotope labeled materials** Marco Evertz[1], A. Kenkel[1], M. Winter[1,2], S. Nowak[1] [1]MEET Battery Research Center, Institute of Physical Chemistry, University of Münster, Germany, [2]Forschungszentrum Jülich GmbH, Helmholtz-Institute Münster, Germany

Short Course Session 1:

Time	Abstr.	A1: **Gary Hieftje** Fundamentals of laser operation	A2: **Johanna Irrgeher** IUPAC Commission on Isotopic Abundances and Atomic Weights (CIAAW): Tables of isotopic composition of the elements and standard atomic weights and their relevance for the plasma sprectrochemist	A3: **Karl Andreas Jensen** Practical approaches to use reaction gases in ICP-QQQ-MS	A4: **Steven J. Ray** Time-of-flight and distance-of-flight mass spectrometry or atomic analyses
15:55-17:40	A1 - A4				

17:40-17:55		**Coffee break, exhibition and poster viewing**

Short Course Session 2:

Time	Abstr.	B1:	B2:	B3:	B4:
17:55-19:40	B1 - B4	**Uwe Karst** Complementary elemental and molecular bioimaging techniques: instrumentation, methods and applications	**Frank von der Kammer** A guide to method development for field flow fractionation analysis of natural and manufactured nanoparticles	**Ilia Roduskhin** Sources of contamination and remedial strategies	**Jacob T. Shelley** Plasma-based ambient desorption/ ionization mass spectrometry
19:40		**Dinner**			
21:00		**Poster viewing and discussions with wine tasting (Bring your own wine)**			

Tuesday, June 12, 2018

Time	Abstr.	
08:00-08:10		**The Nordic Plasma Torch Award** Organising Committee

Session IV: Single particle and single cell analysis by plasma spectrochemistry

Chairman: Michael Sperling

08:10-08:35	O-32	**Analysis of natural and manufactured nanoparticles in complex samples** Frank von der Kammer, University of Vienna, Austria
08:35-09:00	O-33	**How ICP-MS can help to study the fate of engineered nanoparticles in environmental matrices** Carsten Engelhard, D. Mozhayeva, A. Schardt, I. Strenge, B. Spelz Department of Chemistry and Biology, University of Siegen, Germany
09:00-09:25	O-34	**From single particle to single cell ICP-MS: Method developments, achievements, and challenges** Jörg Bettmer, R. Alvarez-Fernández García, M. Corte Rodríguez, S. Cándas Zapico, M. Montes-Bayón Faculty of Chemistry, University of Oviedo, Spain
09:25-09:50	O-35	**Characterization of nanoparticles in food using ICP-MS – How far have we come in the last 10 years?** Katrin Loeschner National Food Institute, Technical University of Denmark, Lyngby, Denmark
09:50-10:05	O-36	**The use of single particle inductively coupled plasma mass spectrometry towards answering real world questions in the energy and chemical industry** Jenny Nelson[1], T. Davis[2], M. Yamanaka[1], V. M. Rodriguez-DeVecchis[3], L. Carbognani Ortega[3], P. Pereira-Almao[3], F. Lopez-Linares[2] [1]Agilent Technologies, Inc., Santa Clara, USA [2]Chevron Energy Technology Company, Richmond, USA [3]Schulich School of Engineering, University of Calgary, Canada

Time	Abstr.	
10:05-10:25		**Coffee break, exhibition and poster viewing**

Session IV continues: Single particle and single cell analysis by plasma spectrochemistry

Chairman: Michael Sperling

10:25-10:40	O-37	**Single cell ICP-MS: the advantages of quantifying the metal content in individual cells** C. Stephan, David Price, R. Merrifield Perkin Elmer Inc., Seer Green, United Kingdom
10:40-10:55	O-38	**Innovations in single particle ICP-MS – accurate detection of pure and alloyed nanoparticles** Chady Stephan, D. Price, R. Merrifield, S. Bazargan Perkin Elmer Inc., Woodbridge, Canada
10:55-11:10	O-39	**Study of the ion cloud formation from gold nanoparticles in ICP-MS by means of microsecond dwell time SP-ICP-MS** Joshua Fuchs[1], M. Aghaei[2], T. D. Schachel[1], M. Sperling[1,3], A. Bogaerts[2], U. Karst[1] [1]Institute of Inorganic and Analytical Chemistry, University of Münster, Germany [2]Research Group PLASMANT, Chemistry Department, University of Antwerp, Belgium [3]European Virtual Institute for Speciation Analysis (EVISA), Münster, Germany

Session V: New analytical capabilities

Chairman: Steve Ray

11:10-11:35	O-40	**Exploration of brain iron balance using stable isotope techniques** Thomas Walczyk[1], C. Jiehua[1], L. Bin[1], N. N. Singh[1], Y. Makino[2], Y. Tanaka[2], T. Hirata[2] [1]Department of Chemistry, National University of Singapore (NUS), Singapore [2]Department of Chemistry, University of Tokyo, Japan
11:35-11:50	O-41	**On-line steel slag analysis with LIBS – a challenge and an opportunity** Arne Bengtson, J. Petersson Swerea KIMAB, Kista, Sweden
11:50-12:15	O-42	**Investigation of extreme natural abundance variation of multiple isotopic systems (B, Zn, Sr, Mo, Nd and Pb) in the North Sea estuary** Johanna Irrgeher[1], A. Reese[1,2], T. Zimmermann[1,2], M. E. Wieser[3], D. Pröfrock[1] [1]Institute of Coastal Research, Helmholtz-Zentrum Geesthacht, Germany [2]Institute for Inorganic and Applied Chemistry, Universität Hamburg, Germany [3]Dept. of Physics and Astronomy, Stable Isotope Laboratory, University of Calgary, Canada
12:15-12:40	O-43	**Double pulse laser ablation ionization mass spectrometry** Andreas Riedo, University of Leiden, The Netherlands
12:40-13:05	O-44	**Challenges and strategies in LA-ICP-MS - from bulk analysis to imaging (and beyond)** Vid Simon Šelih, National Institute of Chemistry, Ljubljana, Slovenia
13:05-13:20	O-45	**Advances in triple quadrupole ICP-MS for environmental and food analysis** Simon Nelms[1], D. Kutscher[2] [1]Thermo Fisher Scientific, Hemel Hempstead, United Kingdom [2]Thermo Fisher Scientific, Bremen, Germany

Time	Abstr.	
13:20-14:20		**Lunch**

Short Course Session 3:

		C1:	**C2:**	**C3:**
14:20-16:05	C1 – C3	**Thomas Walczyk** Tracing element metabolism in animals and humans using stable isotope techniques	**Maryam Aghaei** Modeling an inductively coupled plasma torch by means of FLUENT: Fundamentals and challenges	**Maria Montes Bayon** and **Jörg Bettmer** From speciation to metallomics: Recent analytical approaches and quantification strategies using ICP-MS

|	
16:30	**Excursion to Briksdal Glacier and conference outdoor dinner**

Wednesday, June 13, 2018

Session VI: Radioisotopes and isotopic ratio measurements

Chairman: Yngvar Thomassen

Time	Abstr.	
08:30-08:45	O-46	**Contribution from long-range transport to element distribution in natural surface soils: examples from Norway using ICP-MS** Eiliv Steinnes Department of Chemistry, Norwegian University of Science and Technology, Trondheim, Norway
08:45-09:00	O-47	**Applications of isotopic measurements for determination of long lived radionuclides in the open ocean** Emiliya Vasileva[1], I. Wysocka[1,2], E. Han[1] [1]Environment Laboratories, Department of Nuclear Sciences and Applications, International Atomic Energy Agency, Principality of Monaco [2]Polish Geological Institute, National Research Institute, Warsaw, Poland
09:00-09:15	O-48	**Analysis of uranium using off-line and in-line automated sample preparation techniques for ICP-OES** Charles D. Quarles Jr.[1], B. T. Manard[2], E. M. Wylie[2], N. Xu[2] [1]Elemental Scientific, Inc., Omaha, USA [2]Los Alamos National Laboratory, Los Alamos, USA
09:15-09:30	O-49	**Determination of $^{236}U/^{238}U$ ratios in environmental samples using ICP-MS/MS** Silvia Diez-Fernández[1], C. Bresson[1], F. Chartier[2], O. Evrard[3], A. Hubert[4], H. Jaegler[3], A. Nonell[1], F. Pointurier[4], H. Isnard[1] [1]Den – Service d'Etudes Analytiques et de Réactivité des Surfaces (SEARS), CEA, Université Paris-Saclay, Gif sur Yvette, France [2]Den – Département de Physico-chimie (DPC), CEA, Université Paris-Saclay, Gif sur Yvette, France [3]Laboratoire des Sciences du Climat et de l'Environnement (LSCE), (CEA/CNRS/UVSQ), Université Paris-Saclay, Gif-sur-Yvette, France [4]CEA, DAM, DIF, France

Time	Abstr.			
09:30-09:45		**Coffee break**		
		Short Course Session 4:		
		D1:	**D2:**	**D3:**
09:45-11:30	D1 – D3	**Joanna Collingwood** and **Freddy Adams** Chemical imaging of biological material: X-rays versus plasma methods	**Carsten Engelhard** Nanomaterials characterization by ICP-MS in single particle mode and related techniques	**Heidi Goenaga-Infante** and **Panayot Petrov** Detection, identification and quantification of nanoparticles in complex matrices: Remaining opportunities for hyphenated field flow fractionation
11:30-11:45		**Closing remarks and farewell**		
12:00		**Lunch**		

Poster Presentations

Sunday, June 10 - Wednesday, June 13, 2018

Abstr.

P-1 **CHARACTERIZATION OF CHLORINE IN VEGETABLE OILS BY ICP-MS/MS**
Marine Nicolas[1], Janique Richoz-Payot[1], Stéphane Dubascoux[1], Eric Poitevin[1] and Kornél Nagy[2]
[1] Nestlé Research Center, Institute of Food Safety & Analytical Science, Minerals and Metals group, Vers-chez-les-Blanc, 1000 Lausanne 26, Switzerland
[2] Nestlé Research Center, Institute of Food Safety & Analytical Science, Network Leader/Technology Assessment, Vers-chez-les-Blanc, 1000 Lausanne 26, Switzerland

P-2 **QUALITY ASSURANCE MEASUREMENTS WITH REFERENCE MATERIALS**
Tiina Heikola1, Emmi Myllykylä1, Tiina Lavonen[1]
[1]VTT Technical Research Centre of Finland Ltd, PL 1000, 02044 VTT, Finland

P-3 **INVESTIGATION OF CHEMICAL ELEMENTS REDISTRIBUTION IN PARTICLE VOLUME OF INCONEL 718 POWDER DURING THE PLASMA TREATMENT**
K. Nagulin, R. Nazarov, O. Kudimov, R. Salikhov, A. Gilmutdinov
Kazan National Research Technical University, K. Marx str. 10, 420111, Kazan, Russia

P-4 **INDUCTIVELY COUPLED PLASMA PROCESSING OF NICKEL ALLOYS POWDERS FOR ADDITIVE MANUFACTURING**
K. Nagulin, R. Nazarov, O. Kudimov, R. Salikhov, A. Gilmutdinov
Kazan National Research Technical University, K. Marx str. 10, 420111, Kazan, Russia

P-5 **PLASMOCHEMICAL PROCESSING OF POWDER MATERIALS FOR HEAT-PROTECTIVE COATINGS**
K. Nagulin, R. Nazarov, O. Kudimov, R. Salikhov, A. Gilmutdinov
Kazan National Research Technical University, K. Marx str. 10, 420111, Kazan, Russia

P-6 **NUMERICAL SIMULATION OF THE POWDER PARTICLES BEHAVIOUR IN A TECHNOLIGICAL ICP**
M. Voronov, K. Nagulin, R. Nazarov, A. Gilmutdinov
Kazan National Research Technical University, K. Marx str. 10, 420111, Kazan, Russia

P-7 *ELECTROMAGNETIC NATURE OF VORTEXES IN TECHNOLOGICAL ATMOSPHERIC PRESSURE ICP*
M. Voronov, K. Nagulin, O. Kudimov, A. Gilmutdinov
Kazan National Research Technical University, K. Marx str. 10, 420111, Kazan, Russia

P-8 **COMPARISON OF TWO METHODS FOR DETERMINATION OF IODINE IN FOOD BY INDUCTIVELY COUPLED PLASMA-MASS SPECTROMETRY (ICP-MS)**
Elena Nebera; Svetlana Demidova; Nikita Bardyugov; Alexander Komarov
Russian State Center for Quality and Standardization of Veterinary Drugs and Feeds (VGNKI), 5, Zvenigorodskoe shosse, Moscow, 123022, Russia

P-9 **NEW FRONTIERS IN BIO-MONITORING – TOTAL AND SINGLE PARTICLE ANALYSIS**
Ewa Pruszkowski
PerkinElmer Inc., 75 Nicholson Lane, San Jose, CA 95138, USA

Poster Presentations Cont.

Abstr.

P-10 **LASER ABLATION-HALO-FLOWING ATMOSPHERIC PRESSURE AFTERGLOW-MASS SPECTROMETRY FOR SPATIALLY RESOLVED ANALYSIS OF ACTIVE INGREDIENTS IN PHARMACEUTICAL TABLETS**

Valérie A. Brückel[1], Michael Sperling[1,2], Jacob T. Shelley[3] and Uwe Karst[1]
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[2] European Virtual Institute for Speciation Analysis, Mendelstr. 11, 48149 Münster, Germany
[3] Rensselaer Polytechnic Institute, Department of Chemistry and Chemical Biology, 110 8th Street, Troy, NY 12180 USA

P-11 **ELEMENTAL CHARACTERIZATION ANALYSIS OF DECOMMISSIONING MATERIALS FROM FIR1 TRIGA MARK II TYPE RESEARCH REACTOR**

T. Lavonen[1], T. Heikola[1] and E. Myllykylä[1]
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P-12 **TOTAL ELEMENTAL ANALYSIS OF FOOD SAMPLES WITH ICP-OES AND ICP-MS**

Simon Nelms[1], Shona McSheehy Ducos[2], Daniel Kutscher[2], Tomoko Vincent[2], Nora Bartsch[2]
[1] Thermo Fisher Scientific, Hemel Hempstead, UK
[2] Thermo Fisher Scientific, Bremen, Germany

P-13 **INVESTIGATING ELECTRICAL CONTACT LOSS WITHIN LITHIUM ION BATTERY ELECTRODES BY MEANS OF SINGLE PARTICLE ANALYSIS WITH ICP-OES AND -MS**

S. Wiemers-Meyer[1], M. Winter[1,2], S. Nowak[1]
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[2]Helmholtz Institute Muenster, IEK-12 of Forschungszentrum Juelich, Corrensstrasse 46, Muenster, Germany

P-14 **ANALYSIS OF ORGANOPHOSPHORUS AGING PRODUCTS IN LITHIUM ION BATTERY ELECTROLYTES VIA GC-ICP-SF-MS AND GC-EI-MS**

Yannick Philipp Stenzel[1], Martin Winter[1,2] and Sascha Nowak[1]
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[2] Helmholtz-Institute Münster (HI MS), IEK-12, Forschungszentrum Jülich GmbH Corrensstraße 46, 48149 Münster, Germany

P-15 **SPECIATION OF POTENTIAL TOXIC DECOMPOSITION PRODUCTS IN LITHIUM ION BATTERY ELECTROLYTES BY COMBINATION OF HPLC-ION TRAP TIME OF FLIGHT-MS AND HPLC-ICP-MS**

Jonas Henschel[1], Yannick Philipp Stenzel[1], Martin Winter[1,2], Sascha Nowak[1]
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[2]Helmholtz Institute Münster (HI MS), IEK-12, Forschungszentrum Jülich GmbH, Corrensstraße 46, 48149 Münster, Germany

P-16 **VISUALIZING ELEMENTAL DEPOSITION PATTERNS ON GRAPHITE ANODES FROM LITHIUM ION BATTERIES: A LASER ABLATION-INDUCTIVELY COUPLED PLASMA-MASS SPECTROMETRY STUDY ON FACTORS INFLUENCING THE DEPOSITION OF LITHIUM, NICKEL, MANGANESE AND COBALT**

Timo Schwieters[1,] Marco Evertz[1], Markus Börner[1], Martin Winter[1,2] and Sascha Nowak[1]
[1]University of Münster, MEET Battery Research Center, Institute of Physical Chemistry, Corrensstraße 46, 48149 Münster, Germany
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Poster Presentations Cont.

Abstr.

P-17   **DETERMINING THE MIGRATION OF LITHIUM IN AGED LITHIUM ION BATTERIES BY PERFORMING AN ISOTOPE DILUTION ANALYSIS COMBINED WITH DIFFERENT PLASMA-BASED TECHNIQUES**

Marcel Diehl[1], Marco Evertz[1], Martin Winter[1,2], Sascha Nowak[1]
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[2] Helmholtz-Institute Münster, IEK 12, Forschungszentrum Jülich GmbH, Corrensstraße 46, 48149 Münster, Germany

P-18   **MATRIX-MATCHED STANDARDS FOR GLOW DISCHARGE-SECTOR FIELD-MASS SPECTROMETRY FOR THE ANALYSIS OF LITHIUM ION BATTERY ELECTRODES**

Marco Evertz1, Timo Schwieters[1], Markus Börner[1], Martin Winter [1,2] and Sascha Nowak[1]
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[2] Helmholtz-Institute Münster, IEK-12, Forschungszentrum Jülich GmbH, Corrensstrasse 46, 48149 Münster, Germany

P-19   **A LASER ABLATION ICP-OES METHOD FOR THE INVESTIGATION OF LITHIUM AND TRANSITION METAL DEPOSITIONS FROM LITHIUM ION BATTERY ELECTRODES**

Constantin Lürenbaum[1], Timo Schwieters[1], Marco Evertz[1], Martin Winter[1,2] and Sascha Nowak[1]
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[2] Helmholtz-Institute Münster (HI MS), IEK-12, Forschungszentrum Jülich GmbH, Corrensstraße 46, 48149 Münster, Germany

P-20   **DECIPHERING THE LITHIUM ION MOVEMENT IN LITHIUM ION BATTERIES: DETERMINATION OF THE ISOTOPIC ABUNDANCES OF 6LI AND 7LI VIA HIGH RESOLUTION ICP-OES FOR AGING ANALYSES**

Marcel Diehl[1], Verena Naber1, Yannick Philipp Stenzel[1], Martin Winter[1,2], Sascha Nowak[1]
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[2] Helmholtz-Institute Münster, IEK 12, Forschungszentrum Jülich GmbH, Corrensstraße 46, 48149 Münster, Germany

P-21   **QUANTIFICATION OF DISSOLVED MN2+/3+ IN LITHIUM ION BATTERY ELECTROLYTES BY MEANS OF CE/ICP-MS – A NEW APPROACH FOR THE INVESTIGATION OF TRANSITION METAL DISSOLUTION FROM CATHODE MATERIALS**

Lenard Hanf[1], Andrea Wilken[1], Martin Winter[1,2], Sascha Nowak[1]
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Corrensstraße 46, 48149 Münster, Germany
[2] Helmholtz Institute Münster (HI MS), IEK-12, Forschungszentrum Jülich GmbH, Corrensstraße 46, 48149 Münster, Germany

P-22   **DETERMINATION OF ESSENTIAL AND NON-ESSENTIAL ELEMENTS IN BLOOD SERUM BY Q-ICP-MS**

Agnieszka Nawrocka, Maciej Durkalec, Miroslawa Kmiecik, Aleksandra Paciorek and Andrzej Posyniak
Department of Pharmacology and Toxicology,
National Veterinary Research Institute Al. Partyzantow 57, Pulawy, Poland

Poster Presentations Cont.

Abstr.

P-23   **OFFSHORE WIND CONSTRUCTIONS: CORROSION PROTECTION AS A NEW POTENTIAL SOURCE OF INORGANIC CONTAMINANTS INTO THE MARINE ENVIRONMENT?**

Anna Reese[1,2], Nathalie Voigt[1,3], Tristan Zimmermann[1,2], Johanna Irrgeher[1], Daniel Pröfrock[1]
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[3] Fachhochschule Lübeck, University of Applied Science, Department of Applied Natural Sciences, Mönkhofer Weg 239, D-23562 Lübeck, Germany

P-24   **LEAD ISOTOPE RATIOS FOR POLLUTION SOURCE APPORTIONEMENT IN DIFFERENT COMPARTMENTS OF THE MARINE ENVIRONMENT**

Emilia Vassileva [a], Anna Maria Orani [a] Irena Wysocka[b]
[a] International Atomic Energy Agency, Environment Laboratories, 4 Quai Antoine 1er, 98000 Monaco, Principality of Monaco
[b] Polish Geological Institute National Research Institute, Rakowiecka 4, 00-975 Warsaw, Poland

P-25   **LEAD ISOTOPE RATIOS FOR POLLUTION SOURCE APPORTIONEMENT IN DIFFERENT COMPARTMENTS OF THE MARINE ENVIRONMENT**

Emilia Vassileva [a], Anna Maria Orani [a] Irena Wysocka[b]
[a] International Atomic Energy Agency, Environment Laboratories, 4 Quai Antoine 1er, 98000 Monaco, Principality of Monaco
[b] Polish Geological Institute National Research Institute, Rakowiecka 4, 00-975 Warsaw, Poland

P-26   **ANALYSIS OF ELEMENTS DISTRIBUTION IN THE OMBROTROPHIC PEAT PROFILE BY ICP-MS**

Nikita Sobolev, Konstantin Bogolitsyn, Anna Kosheleva, Alexandr Kozhevnikov, Nikolai Ivanchenko, Sergei Sypalov
Core Facility Center «Arktika», Northern (Arctic) Federal University, 163002, Arkhangelsk, Russia

P-27   **ESTIMATION OF SPATIAL DISTRIBUTION OF PB AND CD IN NORTHERN TAIGA SOIL BY THE METHOD OF ICP-OES**

Nikita Sobolev[a], Irina Kuznetsova[b], Ekaterina Kotova[b], Darya Bedrina[b], Vidas Kriauciunas[b], Alexandr Orlov[b], Kirill Mironenko[a]
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[b] Federal Center for Integrated Arctic Research, 163002 Arkhangelsk, Russia

P-28   **ANALYSIS OF TRACE ELEMENTS DISRIBUTION BY BIOLOGICAL PATHWAYS ON THE TERRITORY OF EUROPEAN RUSSIA ARCTIC USING ICP-MS TECHNIQUE**

Nikita Sobolev[a], Andrey Aksenov[a], Yngvar Thomassen[a,b], Anna Kosheleva[a], Elena Veselkina[a], Valerii Chashchin[a,c], Tatiana Sorokina[a]
[a] Arctic biomonitoring laboratory, Northern (Arctic) Federal University, 163002, Arkhangelsk, Russia
[b] National Institute of Occupational Health, Oslo, Norway
[c] Northwest Public Health Research Centre, St. Petersburg, Russia

P-29   **DETERMINATION OF ELECTRON TEMPERATURE AND CONCENTRATION IN CADMIUM AND ZINC CONTAINING HIGH-FREQUENCY ELECTRODELESS LAMPS**

Zanda Gavare[1,2], Madara Zinge[2], Atis Skudra[2], Egils Bogans[2]
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Poster Presentations Cont.

Abstr.

P-30   **DETERMINATION OF VIBRATIONAL TEMPERATURE OF CN MOLECULE IN THALLIUM CONTAINING HIGH-FREQUENCY ELECTRODELESS LAMPS**

Zanda Gavare[1,2], Madara Zinge[2], Anda Abola[2], Egils Bogans[2]
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[2] Institute of Atomic Physics and Spectroscopy, University of Latvia, 19 Raina Blvd., Riga, LV-1586

P-31   **DETERMINATION OF ARSENOLIPIDS IN BREAST MILK BY HPLC-ICPMS AND HPLC-ESMS**

Mina Martinsen Langfjord[1,2], Chan Xiong[2], Michael Stiboller[2], Elin Lovise Folven Gjengedal[1], Merete Eggesbø[3], Virissa Lenters[3], Kevin A. Francesconi[2]
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[2]Institute of Chemistry, NAWI Graz, University of Graz, 8010 Graz, Austria
[3]Norwegian Institute of Public Health, 0403 Oslo, Norway

P-32   **ARSENIC, BROMINE, AND LEAD IN BREAST MILK AND URINE FROM NORWEGIAN MOTHERS – INTERACTIONS WHICH INFLUENCE THE LEVELS**

Susanne Birkeland[1], Marie Vollseth[1], Sigrun Henjum[2] and Elin Gjengedal[1]
[1]Faculty of Environmental Sciences and Natural Resource Management, Norwegian University of Life Sciences (NMBU), Aas 1433, Norway
[2] Department of Nursing and Health Promotion, Faculty of Health Sciences, OsloMet – Oslo Metropolitian University, Oslo 0130, Norway

P-33   **ANALYSIS OF SILVER NANOPARTICLES IN MUNICIPAL WASTEWATER SLUDGE USING SP-ICP-MS**

Kinnunen V., Perämäki S., and Väisänen A.
Department of Chemistry, P.O. Box 35 FIN-40014 University of Jyväskylä, Finland

P-34   **DETERMINATION OF HEAVY METALS IN POST-PRECIPITATED SEWAGE SLUDGE BY ICP-MS**

Kinnunen V., Reuna S. and Väisänen A.
Department of Chemistry, P.O. Box 35 FIN-40014 University of Jyväskylä, Finland

P-35   **SELECTIVE RECOVERY OF RUBIDIUM USING 3D-PRINTED POTASSIUM COPPER HEXACYANOFERRATE FUNCTIONAL FILTERS**

Enni Nygrén, Elmeri Lahtinen, Siiri Perämäki, Ari Väisänen
University of Jyväskylä, Department of Chemistry, P.O. Box 35, FI-40014 University of Jyväskylä, Finland

P-36   **DEPARTURE FROM THERMODYNAMIC EQUILIBRIUM IN THERMAL PLASMA ARCJET, EMISSION SPECTROSCOPY STUDY**

Alan Mašláni, Viktor Sember, Peter Ondáč, Milan Hrabovský
Institute of Plasma Physics of the CAS, Za Slovankou 1782/3, 18200 Prague, Czech Republic

P-37   **A FIRST COMPREHENSIVE STUDY ON ZINC ISOTOPIC VARIATION OF WATER AND SURFACE SEDIMENT SAMPLES FROM THE ELBE RIVER**

Zimmermann, T.[1, 2], Wieser M. E.[3], Mohamed F. A.[3], Pröfrock, D.[1], Irrgeher, J.[1]
[1] Helmholtz-Centre Geesthacht, Institute of Coastal Research, Marine Bioanalytical Chemistry, Max-Planck Str. 1, 21502 Geesthacht, Germany
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Poster Presentations Cont.

Abstr.

P-38   **DETERMINATION OF ELEMENT PROFILES IN ATLANTIC SALMON SCALES BY LA-ICP-MS**

Claire Peterson, Tonje Fagertun Benden, Rune Pedersen
Norwegian Veterinary Institute, Tungasletta 2, 7047, Trondheim, Norway

P-39   **QUANTITATIVE ANALYSIS OF INORGANIC ARSENIC IN FOOD AND FOOD PACKAGING USING LC-ICP-MS**

Uwe Oppermann[1], Ludivine Fromentoux[1], Jan Knoop[1] and Marcin Frankowski[2]
[1]Shimadzu Europa GmbH, Albert-Hahn-Str. 6-10, D-47269 Duisburg, Germany
[2]Faculty of Chemistry, Adam Mickiewicz University, Poznań, Poland

P-40   **TOWARDS A FUTURE SCREENING METHOD FOR NANOPARTICLES IN SEAFOOD -FOR SURVEILANCE AND RISK ASSESSMENT OF FOOD SAFETY**

Stig Valdersnes[1], Katrin Löschner[2], Berit Solli[1], Tanja Kögel[1], Monica Sanden[1] and Veronika Sele[1]
[1] Institute of Marine Research (IMR), P.O box 1870 Nordnes, NO-5817 Bergen.
[2] Technical University of Denmark (DTU), Kemitorvet 201, 2800 Kgs. Lyngby, Denmark

P-41   **AUTOMATED, HIGH-VOLUME PRECONCENTRATION AND MATRIX REMOVAL SYSTEM FOR ULTRATRACE QUANTIFICATION AND ISOTOPIC DETERMINATION OF TRACE ELEMENTS IN SEAWATER**

Nathan Saetveit
Elemental Scientific, Omaha, NE, USA

P-42   **PERFORMANCE DATA FOR A NEW MULTI-COLLECTOR ICP-MS WITH A MULTI-POLE COLLISION CELL INTERFERENCE REMOVAL DEVICE**

Mark Mills[1], Phil Shaw[1], Yvan Gerard[1], Phil Freedman[1], Andy Burrows[1], Ye Zhao[1] and Bengt Sandgärde[2]
[1]Nu Instruments, Wrexham, United Kingdom
[2]MSNordic AB, Stockholm, Sweden

P-42   **IMPROVED IN-SITU Δ⁷LI ANALYSIS OF SYNTHETIC GLASS BY LA-MC-ICP-MS WITH 1013 Ω AMPLIFIER TECHNOLOGY**

Søren Dalby, Grant Craig[2], Hauke Vollstaedt[2], Nicholas Lloyd[2], Claudia Bouman[2], and Johannes Schwieters[2]
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12   Oral Abstracts

(O-1)
PHYSICS OF TECHNOLOGICAL ICP: BEGINNING OF UNDERSTANDING

A. Gilmutdinov, M. Voronov, K. Nagulin, I. Tsivilskiy

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A plasma chemical reactor, that is based on an atmospheric pressure ICP of a large size and high power (the plasma torch diameter is 8.5 cm and 60 kW power in our case), is used in our laboratory for spheroidization and chemical processing of powders for additive manufacturing. Fundamental properties of this ICP were investigated using an optical plasma diagnostics (plasma imaging by a fast camera) and numerical simulations. A full self-consistent three-dimensional transient model of ICP has been developed. Navier-Stokes equations with a standard k-ε turbulence model were used. These equations have been additionally enriched with two electromagnetic equations. The first one represents the continuity equation of electric potential inside the spiral inductor and results in a spatial distribution of the electric current, that is then used as a source term in the Maxwell's equations. The second set of equations are Maxwell's equations written in a well-known complex form [1] in terms of the magnetic vector potential. All the equations are solved simultaneously at each time step.

An LTE-based two-dimensional stationary model was created as well, that includes influence of both tangential and axial components of the electrical current in the load coil. The axial component allows calculation of the tangential component of the Lorentz forces in the plasma resulting in electromagnetically-driven rotation of the plasma around the axis. The 2D model includes additionally simulation of the powder particles in the plasma. Namely it takes into account calculation of trajectories, heating and evaporation of the particles injected in the ICP, as well as thermal and gas-dynamical load on the plasma from the particles. Having much less computation cost (than the 3D one), the 2D model is useful for relatively rapid multiparameter optimization of the plasma torch to establish a correlation between the operating conditions and the physical properties of the final powder material. This approach will help to obtain a set of conditions for controllable synthesis of composite powders with desired shape, composition and physical properties.

Numerical simulations and high-speed imaging have shown that in contrast to a conventional analytical ICP, significance of the Lorentz forces is much higher in the technological one due to a large size of the torch. In fact, the plasma fluxes in the induction zone are mostly driven by the Lorentz forces. It is the Lorentz force that is responsible for formation of two strong vortexes in the ICP: one vortex rotates in z-r plane of the torch, another one rotates around the axis.

References
V. Colombo, E. Ghedini, M. Gherardi, P. Sanibondi, Plasma Sources Sci. Technol.,   2013, 22, 035010
S. Xue, P. Proulx, M.I. Boulos, Plasma Chemistry and Plasma Processing, 2003, 23, No. 2, 245-263

(O-2)
PLASMA SPECTROCHEMISTRY AND ITS RELATIVES

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"Plasma Science" is an exceptionally broad field; so broad in fact that most scientists involved in it divide themselves along several narrower lines. One such line closely related to plasma spectrochemistry (as practiced by analytical chemists) is "low temperature" plasma science. By "low temperature" is generally meant a plasma with an average energy below 1 eV, a value that corresponds in temperature to 11,600K. Thus, glow discharges, Ar ICPs, barrier discharges, flowing afterglows, dc arcs, and high-voltage sparks would all be viewed as low-temperature plasmas.

Recently, a biennial review on this topic was published* and reveals the scope of this area of science and technology. Ways of generating low-temperature discharges, their fundamental characteristics, and their applications are all covered. Plasmas very similar to those described at this year's Nordic Conference are employed for such diverse applications as wound healing, sterilization, synthesis of nanoparticles and other novel materials, surface preparation and, of course, analytical chemistry and measurement science. The coverage consists of a large number of short (~two pages) sections, each of which deals with a specific topic.

Included specifically in this review is a section on low-temperature plasmas for analytical chemistry. Present in this section is a summary of work on fundamental understanding and modelling of analytical plasmas such as the Ar ICP and glow discharge, and a description and evaluation of new plasma sources used for chemical analysis, including LIBS, Laser-Ablation Molecular Isotope Spectroscopy (LAMIS), plasma filamentation, the flowing atmospheric-pressure afterglow (FAPA), solution-cathode glow discharge (SCGD), and the Microwave-supported Inductively Coupled Atmospheric-pressure Plasma (MICAP). Recent work with most of these plasmas will be described in several lectures at the current Nordic Conference on Plasma Spectrochemistry, and the present author earlier described studies on several of them. Indeed, at the 2016 Nordic Conference, he emphasized investigations into the SCGD and MICAP; recent work with both sources will be included here.

* J. Phys. D: Appl. Phys. 45 (2012) 253001 (37pp)

(O-3)
PHYSICS OF SPECTROANALYTICAL ICP: FINALIZATION OF UNDERSTANDING

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Historically spectroanalytical Inductively Coupled Plasma (ICP) was developed and optimized first for optical emission analysis. Then the existing ICP sources were applied for mass-spectral analysis (ICP-MS) almost without changes. Therefore the ICP ion source still needs to be optimized for ICP-MS. Particularly, it is experimentally [1] and theoretically [2] shown that the presence of the mass-spectrometer interface affects the plasma flow pattern significantly. Therefore an experimentally proven numerical model of ICP-MS is necessary, that allows prediction the plasma behavior in variety of operating conditions. Overwhelming majority of the existing simulations of ICP-MS deal with the plasma in the atmospheric pressure part of the ICP-MS interface. To the best knowledge of the authors, only group of Spencer *et al* has a model of plasma behind the MS sampler [3]. This is a stationary two-dimensional model and should be therefore further improved. Our work presents a numerical model of 3D transient gas flow inside the ICP torch connected to a mass spectrometer interface. The model includes the plasma in the ICP torch and propagation of the plasma through the sampler until the MS skimmer. Results of the simulation provide spatial and temporal distributions of temperature, pressure and velocity in details.

The developed model is based on our previous simulations of a free burning plasma used in ICP-AES. It takes into account the design of a real ICP-MS system, turbulent flow of argon, and electromagnetic heating of the argon. The heat source has a toroidal form and was simulated separately using a fully self-consistent stationary ICP model. Therefore the presented model does not take into account the gas ionization, but provides a comprehensive data on supersonic gas flow pattern inside the ICP torch and the vacuum ICP-MS interface. Results of simulations of the temperature and the velocity in the supersonic flow after the sampler cone has been compared to the experimental works of Spencer *et. al.* [4].

Numerical simulations have the first time revealed a rapid periodical deflection of the supersonic jet inside the MS-interface along the walls of the sampler cone that is caused by the asymmetrical rotation of the plasma injection. This rotation is visualized by a high-speed camera. The number of "Mach diamonds" formed by the shock waves during propagation of supersonic gas jet inside the interface varies for cold and heated gas conditions.

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(O-4)
PARTICLE TRANSPORT IN THE ICP TORCH: WHAT MODELING REVEALS?

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An inductively coupled plasma, connected to a sampling cone of a mass spectrometer, is computationally investigated. In the 2D axisymmetric ICP-MS model, we first obtain stable plasma properties for Ar in the so-called continuous phase model (CPM), i.e. for the plasma temperature and electron density and for the gas flow behavior. Subsequently, we introduce the sample particles into the ICP with the discrete phase model (DPM). During each iteration, we calculate the exchange of mass, momentum and energy between plasma and particles, and we update the DPM and CPM. When convergence is reached, we can track the particles to determine their position, their phase (liquid or vapor), velocity and temperature, as well as the ionization of the vapor atoms [1-3].

We investigated the introduction of different elemental particles (i.e., copper, zinc, and gold) in an inductively coupled plasma torch. The spatial position of the ion clouds inside the torch as well as detailed information on the sample species fluxes at the position of the sampler orifice and the exhausts of the torch are provided. Indeed, due to different boiling and ionization temperatures as well as different viscosity and diffusion of different materials, the position at which the sample or sample cloud may move in the radial direction to the outer region and get further away from the central channel is different. Hence, this study enables us to learn to what extent these differences affect the ion cloud transport towards sampler cone [4-5]. More specifically, particles are injected with different sizes in order to find in which range a complete evaporation and ionization inside the torch can be guaranteed. Studying the radial diffusion, the effect of on- and off-axis injection is also studied. We clearly show that the ion clouds of on-axis injected material are located closer to the sampler with less radial diffusion. This guarantees a higher transport efficiency through the sampler cone. Moreover, our model reveals the optimum ranges of applied power and flow rates, which ensure the proper position of ion clouds inside the torch, i.e., close enough to the sampler to increase the fraction that can enter the mass spectrometer and with minimum loss of material toward the exhausts as well as a sufficiently high plasma temperature for efficient ionization. Recently, a direct comparison with experiment is performed in order to find the optimum size of gold nano-particles at a certain operating condition [6].

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(O-5)

ATMOSPHERIC-PRESSURE PLASMAS AS IONIZATION SOURCES FOR ATOMIC, MOLECULAR, AND BIOLOGICAL MASS SPECTROMETRY

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Analytical plasmas, which operate at ambient pressures, and mass spectrometry have been in a symbiotic relationship since the near-coincident advent of the inductively coupled plasma (ICP) ionization source and atmospheric-pressure inlets. Preceding that discovery by only a few years, it was shown that low-power plasmas could be used for soft ionization of intact molecules through atmospheric-pressure chemical ionization (APCI) pathways. More recently, analytical plasma source development has seen a resurgence with the realization of a variety of low-power atmospheric-pressure plasma designs useful as MS ionization sources. Interest in such plasmas has also been fueled by the advent of ambient desorption/ionization mass spectrometry (ADI-MS), which aims to reduce or eliminate sample preparation. Of the many ADI-MS sources, AP plasmas are unique in that they have the ability to create a wide-range of energetic species useful for desorption and/or ionization processes.

Plasmas produce highly energetic species (e.g., ions, metastable neutrals, fast electrons, etc.), which can lead to high-energy physical or chemical processes to fragment and ionize molecules. This fragmentation can be so extensive that molecules are broken down into bare elemental constituents. In addition, low-energy ionization reactions can also occur due to the abundance of collisional cooling that can take place at ambient pressures. For instance, the helium-based flowing atmospheric-pressure afterglow (FAPA) source has been shown to produce intact molecular ions of molecular species with quite high ionization efficiencies.

This presentation will demonstrate the broad utility and range of applications of low-power atmospheric-pressure glow discharges (APGD), specifically the FAPA discharge, and the solution-cathode glow discharge (SCGD). The possibilities of these devices extend well beyond conventional atomic and small molecule detection. By tuning the chemistry of the discharge, we can alter conventional ionization modes to encompass elemental analysis to biomolecular detection to polymer analysis. For instance, our group has developed a method to detect elemental ions with FAPA-MS via online complexation reactions with volatile ligands. But, the open-air nature of FAPA can produce isobaric interferences from ambient species. To overcome this issue, differential mobility spectrometry was used as a post-ionization filter to remove background ions. Ultimately, FAPA-DMS may dramatically improve selectivity and sensitivity in fieldable MS applications. Meanwhile, it was found that SCGD-MS could be used for the detection of atomic, molecular, and biological species directly from solutions. Furthermore, it was found that peptides could be tunably fragmented at atmospheric pressure, which led to 100% sequence coverage for many of the peptides examined.

(O-6)

A NEW GENERATION OF SOLID-STATE DETECTORS FOR MASS SPECTROMETRY

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The ion detection strategies used in mass spectrometry have evolved over many decades, but still fall into two general categories. Ion detection by electron multiplication, such as occurs in microchannel plate (MCPs) or continuous electron multipliers (CEMs), provides single-ion detection capability, is very rapid, convenient, and consequently is used widely. However, such detection systems are also fundamentally limited in the precision of measurements by dynode statistics, and show a limited mass-range of ions that can be detected. Ion detection by direct charge integration, as practiced in Faraday cup ion detectors, is a tried-and-true method of ion detection. Sophisticated modern Faraday-based ion detectors do not suffer from the complications posed by dynode statistics, but are also much slower and less sensitive than the electron-multiplication approaches. Both of these approaches are also predominantly used as single-channel detection approaches.

Recently, advanced semiconductor ion detectors have been developed as a means to address these limitations and extend ion detection capabilities for mass spectrometry. Here, a sixth-generation focal plane camera (FPC) ion detector is evaluated. The FPC is a monolithic semiconductor-based application-specific integrated chip, capable of direct charge integration of ions that are neutralized upon striking one of an array of Faraday-strip electrodes. Each ion detection Faraday-strip is connected to a dedicated current-integrator circuit etched within the supporting silicon wafer of the chip, and the entire array of 1704-individual electrode channels is under computer control. As a consequence, each detection channel can be controlled and accessed individually. This strategy introduces new capabilities to mass spectrometry detection, such as non-destructive readout, automatic detector gain control, and random channel access. As importantly, direct charge integration shows no mass bias and is thus equally useful on both positive or negative ions of large or small m/z. Here, a new 1704-channel FPC, developed for use with distance-of-flight mass spectrometry, will be introduced and evaluated.

(O-7)

DIRECT SAMPLING AND ANALYSIS OF AIRBORNE PARTICULATE ORGANIC MATTER BY PROTON-TRANSFER-REACTION MASS SPECTROMETRY

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Particulate organic matter in the Earth's atmosphere is difficult to measure, especially if analytes are reactive and/or semivolatile. Any technique based on particle collection onto a substrate (*e.g.*, Teflon or quartz filters) will generate sampling artefacts due to surface reactions and ad- and desorption of semivolatiles. Online sampling without sample pre-collection, as for example implemented in the aerosol mass spectrometer (AMS), has greatly reduced sampling artefacts. AMS measurements of organic analytes do, however, suffer from the drawback that molecular-level information is, in most cases, lost during particle vaporization at 600 °C and hard (70 eV electron) ionization.

Proton-Transfer-Reaction Mass Spectrometry (PTR-MS) is a well-established online measurement technique for gas-phase organics. Soft ionization via gas-phase hydronium ions (H_3O^+, generated in a plasma ion source) preserves, to a large extent, molecular-level information and thus allows identifying organic compounds at an elemental composition level. We have recently developed a particle inlet system for PTR-MS instruments (Eichler et al., 2015). The CHARON ("*Chemical Analysis of Aerosol On-line*") inlet consists of a gas-phase denuder, an aerodynamic lens and a thermodesorption unit. The activated carbon monolith denuder removes gaseous organics from the sampling flow. The aerodynamic lens enriches the particle concentration in the instrument subsampling flow, which is heated before introduction into the PTR-MS instrument. A temperature of ~150 °C is used for particle vaporization.

The CHARON-PTR-MS system has been successfully used for investigating organic particle emissions from a marine diesel engine (Eichler et al., 2017) and for characterizing ambient organic aerosol in three European cities (Müller et al, 2017). These measurements have demonstrated that the CHARON PTR-MS system generates online and real-time elemental composition information on particulate organic matter in or emitted to the atmosphere. Selected application examples will be shown.

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(O-8)

RECENT SPECTROCHEMICAL EMERGING ADVANCES APPLICATIONS IN ENVIRONMENTAL MONITORING

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Environmental monitoring of the elements has been traditionally carried out by manual sampling and stationary laboratory instrumentation. In controlled laboratory conditions, ICP-OES and ICP-MS instrumentation are robust and routinely used in elemental analysis from various matrices. Analytical performance of these instruments is high and low uncertainty estimates are typical. Maintenance costs of ICP-instrumentation can be high but higher throughput laboratories can run at satisfactory cost/sample level.

From environmental monitoring point of view there are several challenges and drawbacks in current analytical data production procedure such as the uncertainty of sampling and logistics process; in most cases uncertainty is unknown which decreases the value of data produced. Another aspect is that there is also long time period between sampling and obtaining the actual analysis result. As far as decision making is concerned, there is an urgent need in environmental monitoring for instruments and monitoring systems which could provide continuous analytical data real-time. Monitoring of aquatic environment is typical such application where authorities or industrial facility operators would like to track continuously certain elemental concentration levels. Such elemental analytical fingerprints could provide data for decision making about the actual sources and indicate possible sudden spills and transient phenomena by various plants and agricultural areas. To overcome the challenges and to meet the new emerging requirements in environmental monitoring, various scientific and technological experiments has been carried out over the last decades related to on-line analysis of elements in aquatic environment by ICP, spark discharge excitation or LIBS. So far there has been no technological or commercial success of routine and robust monitoring system.

Just recently, a novel spark optical emission micro plasma technique has been successfully demonstrated in environmental monitoring application for elemental analysis. In addition of sampling unit, the system consists of high energy spark unit which generates stabile plasma without the use of shield gas. With current optical arrangement, detection levels of 0.1 ppb has been obtained for several elements. The system enables continuous in-situ measurements with low running costs. Latest results and description of remote operation of the instrumentation in aquatic environmental monitoring will be presented.

(O-9)

FLOWING ATMOSPHERIC PRESSURE AFTERGLOW FOR IONIZATION IN ELECTROCHEMISTRY/MASS SPECTROMETRY

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The prediction of a drug's metabolism is a crucial factor in drug development. Besides well-established in vitro and in vivo methods using biological matrices, several biomimetic models have been developed in the past decades. One approach is the application of electrochemistry (EC) for the study of oxidative metabolism reactions. Electrochemistry coupled on-line to mass spectrometry (MS) allows the fast screening of xenobiotics with respect to labile sites in the molecular structure and can mimic the formation of potential metabolites. Conventionally, electrospray ionization (ESI) is used for EC/MS hyphenation, while non-polar substances have been analyzed by means of atmospheric pressure chemical ionization (APCI) in the past.[1]

In 2013, Pfeuffer *et al.* introduced a new ADI-MS source called halo-flowing atmospheric pressure afterglow (halo-FAPA).[2] Here, molecules are desorbed/ionized in the afterglow region of a halo-shaped atmospheric pressure glow discharge sustained in helium. Due to the ionization chemistry of halo-FAPA-MS, molecules of a broad range of polarities in the relatively low mass range (*e.g.*, under 1000 Da) can be detected in very low amounts (*ca.* 100 amol). This versatility makes the FAPA ionization source an interesting alternative to standard methods for several hyphenated MS techniques and EC/MS in particular, since the polarity of different xenobiotics and their resulting oxidation products can differ significantly. Nevertheless, only one report on the hyphenation of FAPA and EC/MS exists to date.[3]

In this work, an EC/FAPA-MS hyphenation was developed and the scope of this technique was investigated by analyzing two different substance classes of very different polarities. Both substance classes, namely phenothiazines and polycyclic aromatic hydrocarbons (PAHs), are of relevance for pharmaceutical and environmental research and have previously been studied via EC/MS with ESI and APCI, respectively. Mass voltammograms were obtained for a large number of substances by use of an automated EC/MS setup, where potentials between 0 and 2.5 V *vs.* Pd/H$_2$ were applied to an electrochemical flow-through cell equipped with a boron-doped diamond (BDD) working electrode. The effluent from the cell was fed online into a heated nebulizer and the generated aerosol was ionized by a FAPA ionization source. Generated ions were detected *via* high resolution mass spectrometry (HRMS) with an orbitrap mass analyzer.

Especially for the highly non-polar PAHs, ionization in the FAPA proved advantageous with respect to sensitivity (*e.g.*, *ca.* 50-fold increased signal intensity for Benzo[a]pyren and its oxidation products compared to APCI). But also for the investigated phenothiazines, the results obtained with the two methods were comparable. Thus, FAPA ionization proved to be a valuable tool for enhancing the versatility of metabolism studies *via* EC/MS.

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(O-10)

QUANTITATIVE BIOIMAGING BY LA-ICP-MS AS A TOOL TO SUPPORT TOXICOLOGICAL AND MEDICAL INVESTIGATIONS

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Laser-ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) provides sensitive elemental detection with a spatial resolution down to the low µm range. By using thin tissue sections for bioimaging, quantification is possible by using external calibration with matrix-matched standards. The obtained quantitative distribution maps of target elements provide important information about the transport, metabolism and distribution of these elements between different organs, organ structures, tissue types down to cell types. Such information is crucial in medical investigations and toxicological studies related to elemental species such as metabolic disorders related to metal species, metallodrugs used in chemotherapy, metal species used as contrast agents in diagnostic imaging or exposure to metal and metal oxide nanoparticles. Here we report about the possibilities of bioimaging by LA-ICP-MS to support such investigations by providing valuable information improving our understanding of interactions and mechanisms targeting at improved diagnostic and therapeutic efficacy. Requirements for sample preparation and quantification will be discussed as well as possibilities and remaining challenges in this field.

(O-11)

VISUALIZING ELEMENTAL DEPOSITION PATTERNS ON GRAPHITE ANODES FROM LITHIUM ION BATTERIES: A COMBINATION OF LASER ABLATION-INDUCTIVELY COUPLED PLASMA-MASS SPECTROMETRY AND LASER ABLATION-INDUCTIVELY COUPLED PLASMA-OPTICAL EMISSION SPECTROMETRY

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Lithium-ion batteries, first introduced by Sony in 1991, still experience a loss in performance over time. Although the technology is state of the art in portable consumer electronics, widespread application in automobiles demands improvement beyond the current capabilities. Understanding deterioration processes and mechanisms (the so called aging) requires the examination of aged cells. As electrochemical cells and especially electrodes do not age homogeneously and electrochemistry in general is heavily dependent on surface properties, bulk analysis is not suitable for investigating these phenomena. However, the understanding of these aging phenomena in Lithium Ion Batteries (LIBs) is a crucial factor for current and future LIBs. Even state of the art LIB systems show some degree of performance loss over time which has to be investigated. For example, changes in the distribution of lithium or transition metal deposition in the LIB can have a huge impact on the cycle and calendar life of cells.

Therefore, we developed methods using laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) and laser ablation-inductively coupled plasma-optical emission spectrometry (LA-ICP-OES). The solid samples were investigated using a 193 nm ArF Excimer and a 213 nm Nd:YAG Laser, respectively.

Due to a lack of commercially available solid standard materials and to minimize the mentioned influences we developed solid standard materials with a known content of analytes which are matrix matched. The investigations were carried out by visualizing the ^{7}Li and TM patterns (^{60}Ni, ^{55}Mn and ^{59}Co) of whole coin and pouch-bag electrodes.

(O-12)

ELEMENTAL BIOIMAGING AND SPECIATION ANALYSIS TO TRACK GADOLINIUM FROM MRI CONTRAST AGENTS IN THE BRAIN

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Metallopharmaceuticals find increasing use as therapeutics and as diagnostic agents in recent years. While platinum-based cytostatics likely are the most important examples, gadolinium-based magnetic resonance imaging (MRI) contrast agents have become a focal point of researchers and governmental agencies in the last decade. The compounds are known to be tolerated well, and to exhibit only few side-effects due their fast excretion kinetics with a half-life of only two hours. However, in 2006, these compounds started to be associated with a newly discovered disease, nephrogenic systemic fibrosis (NSF), which is only observed for dialysis patients. Furthermore, the disease has only been described for contrast agents with linear ligands, but not for those with macrocyclic ligands. This indicates an influence of the lower kinetic stability of the contrast agents with linear ligands. While the general cause of the disease with a deposition of the gadolinium in the lower parts of the skin has been identified, many details of the pathogenesis are still unknown. Very recently, small residues of the contrast agents have been discovered to remain in the human brain, and many related questions are currently under investigation. Even despite any current indication for respective pathogenic effects, scientists, manufacturers and regulatory agencies are concerned about these findings. To investigate this situation, liquid chromatography (LC) coupled to inductively coupled plasma-mass spectrometry (ICP-MS) and electrospray mass spectrometry (ESI-MS) are used, combined with spatially resolved analysis by laser ablation (LA)-ICP-MS imaging.

In this lecture, the development of the respective analytical methods and their application to address the challenges raised above are presented.

(O-13)
COMPLETING THE JIGSAW: MULTI-MODAL APPROACHES TO INVESTIGATE BRAIN IRON IN HEALTH AND DISEASE

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This talk will focus on the analytical challenges associated with investigating brain iron metabolism in health and disease, with a particular focus on Alzheimer's and Parkinson's disease. The use of plasma methods to investigate iron in brain tissue will be placed in context with other complementary methods, including synchrotron X-ray methods for subcellular sub-ppm analyses of the distribution and mineral forms of iron in postmortem tissues, and clinically applicable Magnetic Resonance Imaging methods to study brain iron distribution and concentration in the living human brain. The evaluation of iron in the substantia nigra in Parkinson's disease, and the chemically reduced iron associated with amyloid plaques in Alzheimer's disease, will be used as case studies.

(O-14)

QUANTIFICATION OF METALLOPROTEINS RELEVANT TO HUMAN HEALTH USING COMPLEMENTARY HYPHENATED TECHNIQUES AND ISOTOPE DILUTION ICP-MS

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The accurate determination of metalloproteins and metal-protein complexes is crucial in clinical and biomedical analysis, as they are being increasingly used as important biomarkers for diseases, the control of treatments efficiency or for drugs development control[1]. Plasma metal-protein complexes, and in particular, metallo-complexes with transferrin and albumin have been the subject of many research papers because of their potential involvement in the diagnosis and treatment of critical diseases such as Cancer and Neurodegenerative (ND) diseases.

Several strategies for the fractionation of plasma metal-protein complexes based on the use of size-exclusion, anion-exchange and reverse phase chromatography have been reported previously. Relatively poor chromatographic selectivity and/or poor recoveries have been reported for metallo-complexes with albumin and transferrin using size-exclusion chromatography[1]. Successful ion exchange methodologies[2], have been associated with long analysis times and problems caused by the introduction of high-salt elution buffers into the ICP-MS. Strategies based on reversed phase chromatography separations have been shown to cause destruction of labile metal-protein complexes due to the use of ion pairing reagents and/or high content of organic solvents. As an alternative to particle-packed columns, monolithic chromatographic separations have been demonstrated to offer improved performance in terms of chromatographic selectivity and significantly reduced time of analysis compared with previously reported ion-exchanged methodology for plasma metal-protein complexes in cancer applications[3]. More recently, the potential of field-flow-fractionation has been demonstrated for the non-denaturing gentle separation of transferrin and albumin standards[4].

This lecture will discuss the potential of the complementary use of field-flow fractionation (FFF) and monolithic chromatography with isotope dilution (ID) ICP-MS for the detection, and accurate quantification of metal adducts/complexes of plasma proteins relevant to cancer and ND applications. Main focus will be on adducts of carboplatin with plasma proteins, in particular, with albumin, which we have found to account for approximately 85% of the Pt in drug-incubated blood, demonstrating that such adducts are key competitors for the drug binding to DNA in cancer models. Reference methodology based on the use of species-specific isotope dilution calibration has been developed and validated. In this context, FFF was found to be particularly useful to provide detailed information on the formation of different adduct isoforms during optimisation of conditions for calibrant and spike production (e.g. by incubation of the individual proteins with either, natural or [194]Pt-enriched carboplatin). Further separation improvements needed for metalloprotein quantification in small complex matrices relevant to ND research will be highlighted. The lecture will also discuss the main contributing factors to the overall measurement uncertainty and the importance of the achievements presented here for the provision of reference values to human cancer trials and for underpinning measurements in ND research.

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(O-15)

ELEMENTAL LABELLING AS A GENERAL PLATFORM FOR ICP-MS ANALYSIS OF CLINICAL BIOMARKERS

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Iron plays a fundamental role in cell life and its concentration in living organisms is precisely regulated. Different molecules for iron storage and transport are used to maintain its intracellular homeostasis which is often altered in cancer cells. Specifically, recent studies have demonstrated that in breast cancer cells, the expression/activity of several iron-related proteins is deregulated and that these alterations may have a prognostic impact in patients with breast cancer. For instance, recent reports have shown that the labile iron pool is increased in breast cancer cells compared with normal breast epithelium. This finding supports observations dating from the 80s by which TfR1, a cell surface receptor responsible for transferrin-mediated iron uptake, is upregulated in many cancers. On the other hand, ferritin which is an intracellular Fe storage protein whose main function is to sequester excess ferric iron and thus preventing high concentrations of soluble ferric iron from being toxic to cells, has been also studied in combination to breast cancer diagnosis.

Thus, in order to obtain quantitative information of all these parameters that permit to compare breast cancer cell lines of different malignancy, sensitive and absolute analytical strategies have to be developed. In this regard, the use of element-tagged immunoassays have been applied for protein detection and quantification based on the capabilities exhibited by inductively coupled plasma mass spectrometry (ICP-MS) for sensitive and selective elemental detection [1]. Thus, element-tagged immunoassays, which combine the sensitivity of ICP-MS and the specificity of an antibody, have been successfully applied to different analytical problems. In this work, we evaluate the development of different ICPMS linked immunoassays to permit the quantification of ferritin (and Fe:ferritin ratios), transferrin and transferrin receptor 1 in breast cancer cells of different malignancy. In this regard, elemental labelling using metal chelates or direct derivatization reactions (e.g. iodination) will be addressed.

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(O-16)
QUANTITATION OF PEPTIDES BY SELENIUM LABELING

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Peptides are attractive as drug compounds as they usually offer high selectivity, high efficacy and low toxicity. However, formulation and delivery of peptides, are important to consider in the development, and analytical methods with adequate selectivity and sensitivity are required.

Recently, selenium (Se) was suggested as an elemental label allowing for easy and sensitive quantification in biological matrices by LC-ICP-MS. The Se-label may be introduced by exchange of a sulfur (S) containing amino acid with a Se-containing analogue or simply by adding a Se-containing amino acid to the sequence [1].

The aim of this study was to develop a method for quantification of peptides in biological samples, like plasma, using the cell penetrating peptide penetratin (Pen) and its selenium labelled analogue (PenMSe) as model peptides. The method should include removal of plasma proteins, separation by reversed phase UHPLC, detection by S- and Se-based LC-ICP-MS/MS and quantitation by post column isotope dilution analysis (IDA).

Validation of the Se-based and S-based method was performed in both human plasma and aqueous solution. The Se-based quantification showed high selectivity and sensitivity and low detection and quantification levels were observed. The S-based quantification was possible as well. A comparison of Se- and S-based detection will be addressed, including benefits and drawbacks of Se-labelling regarding analytical figures of merit and peptide stability.

[1] L.H. Møller, J.S. Bahnsen, H.M. Nielsen, J. Østergaard, S. Stürup, B. Gammelgaard, Selenium as an alternative peptide label – comparison to fluorophore-labelled penetratin, European Journal of Pharmaceutical Sciences, 67 (2015) 76-84.

(O-17)

ARSENIC SPECIATION ANALYSIS ELUCIDATES THE RISK ASSESSMENT OF FOOD SUPPLEMENTS WITH INGREDIENTS OF MARINE ORIGIN

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Many potential health benefits are related to the consumption of marine organisms due to the presence of high amounts of beneficial bioactive compounds (e.g. polyunsaturated fatty acids, various peptides, minerals …). Therefore, these organisms are frequently used as base for several food supplements (FS). On the other hand, marine organisms are also known to contain high levels of arsenic (As), resulting in elevated As concentrations in FS with ingredients of marine origin, such as fish oil, krill oil or algae. Since human health risks are not related to the total As concentration but are species dependent, analysis of the relevant toxic As species in FS is mandatory for a correct risk assessment.

The aim of the present study was to make an exposure and risk assessment of As (species) resulting from the consumption of these types of FS, based on 60 samples collected in a Belgian market study. In this context, the determination of the most toxic fraction, inorganic arsenic (As_i) and the non-toxic fraction arsenobetaine (AB) is particularly important. In addition, we considered the 'potentially toxic As fraction' i.e. 'As_{tot}-AB', consisting of not only As_i, but also As species with unknown toxicity, such as arsenosugars and arsenolipids which can occur in marine matrices, in particular in algae.

Analysis of As_i in algae by HPLC-ICP-MS is complicated by the presence of arsenosugars in these organisms. Routine methods for As_i analysis in terrestrial matrices do not automatically guarantee a separation of As^V and arsenosugars. The objective of this study was to optimize and validate a method to ensure a correct quantification of methylarsonate (MA), dimethylarsinate (DMA), AB and As_i in marine matrices. Arsenobetaine could not be determined on the same anionic column as the other species, therefore a method using a cationic column was needed to separate AB from other uncharged or cationic species.

Exposure to As_i, MA, DMA and 'As_{tot}-AB' was calculated for each sample by multiplying the concentration of these compounds with the maximal recommended dose of the FS. Risks related to the intake of arsenic species in the food supplements were evaluated by comparing the calculated exposure to selected acute and (sub)chronic reference values. For As_i, a distinction was made between the general Belgian population and a sensitive population group, i.e. persons with an increased cancer risk. For the latter group a more severe reference value was applied. The risk evaluation for the chronic intake of As_i and the potentially toxic As fraction was carried out by calculating a margin of exposure (MOE), whereby MOE values > 100 were considered as 'of concern'. Regarding MA and DMA no (sub)chronic risk was present, and no risk for acute toxicity of As_i was detected either. The intake of As_i was only of concern for sensitive groups in the case of chronic consumption of 24% of the tested FS based on algae. The intake of the potentially toxic As fraction was of concern in the case of chronic consumption of 19% of the tested food supplements based on algae, 6% of the tested food supplements based on fish oil and 67% of the tested food supplements based on krill oil.

These findings illustrate the need for more information regarding the toxicity of the potentially toxic arsenic species (mainly arsenosugars and arsenolipids), starting with a correct characterization of these species.

(O-18)

SURVEY OF ARSENIC SPECIES IN THE TOP 10 MOST CONSUMED SEAFOODS IN THE US

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A survey was conducted to determine the levels of arsenic species in commonly consumed seafood in the U.S., as well as to further verify performance of a newly developed and validated method on a relevant sample set. Samples were selected based on the annual Top Ten seafood list from the National Fisheries Institute, and were collected from supermarkets in Maryland, Kansas and California. In some cases (shrimp, salmon, clams crab and canned tuna), multiple species were obtained to better represent a category (e.g. snow crab, blue crab, Dungeness crab). Samples were analyzed for 16 arsenic species, as well as total non-polar arsenic. Arsenobetaine represented the vast majority of arsenic, inorganic arsenic levels were quite low, and non-polar and arsenosugar levels varied widely. Though not a statistically rigorous sampling, these results nevertheless represent the most comprehensive study to date of arsenic species in the U.S. diet from seafood consumption.

(O-19)

FAST ARSENIC SPECIATION ANALYSIS OF WINE, AND RICE BY LC-ICP-QQQ

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Arsenic (As) is a ubiquitous element, that is naturally present in the environment, but also as a consequence of human activity. It is well known that As toxicity depends on the chemical form, being inorganic arsenic species (AsV and AsIII) more harmful than the organic forms of this element. There is a big concern with dietary exposure to arsenic, and particularly rice is one of the main sources of arsenic in nutritional intake. Some governments have already set limits for inorganic arsenic in food, and some others are in the process of doing it. For instance, China allows a maximum limit of 150 ng/g of inorganic As in rice, whereas the EU regulation range between 200-300 ng/g of inorganic As for rice-based products for adults, and 100 ng/g for infants. The FDA has proposed an action level for inorganic As concentrations higher than 100 ng/g in infant rice cereal. Infants are more vulnerable to As content in food because of their lower body weight, and so, infant food should be taken into special consideration.

Usually, speciation methods for arsenic consisted on the separation of the individual species by ion exchange high pressure liquid chromatography hyphenated with inductively coupled plasma – mass spectrometry (HPLC – ICPMS), and inorganic arsenic was expressed as the addition of the AsIII and AsV species. In the method here proposed AsIII was intentionally oxidized to AsV with hydrogen peroxide prior to analysis, allowing all inorganic arsenic to be expressed as AsV. Separation took place in an Agilent 1260 HPLC, using a narrow bore, small particle column. That allowed the inorganic As to be separated from monomethylarsonic acid and dimethylarsinic acid in less than 2 minutes. This analysis is 10 times faster than the current Food and Drug Administration method for As speciation. The determination of As was conducted in an Agilent ICP-QQQ in reaction mode, using O2 to create the AsO+ species, that was measured at m/z 91 free of interferences. The injection of small volumes also helped to mitigate non-spectral interferences like carbon enhanced ionization.

The current method was applied to wine, rice, and rice products, to prove robustness with different matrices. Validation studies were conducted from two different laboratories and results of the method's accuracy, and reproducibility are presented here.

(O-20)
SELENIUM SPECIATION IN FEED BY HPLC-ICP-MS

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Selenium is an essential nutrient for both humans and animals, however at higher concentrations selenium can be toxic. Organic selenium species, incorporated in proteins, are more effectively taken up by the body than inorganic selenium. Therefore, selenized yeast is often added to feed, providing a source of organically bound selenium.

Addition of selenium to feedingstuffs is limited to a maximum concentration of 0.5 mg total Se/kg feed and a maximum of 0.2 mg organic Se/kg feed (EU 2015/489). To control whether feedingstuffs comply with this legislation there is a need for a method to discriminate between different selenium species. Elemental speciation is commonly performed by online coupled HPLC-ICP-MS.

This approach was used for selenium speciation as well. We have developed a method for the separation of the most common selenium species using HPLC-ICP-MS. The anion exchange method separates the organic species selenomethionine, selenocysteine and seleno-DL-cystine. The inorganic species selenite and selenate are included in the method as well. Sensitive ICP-MS analysis of selenium species is difficult because of the relatively high ionization potential and the presence of many interferences. The detection of selenium by DRC was optimized using methane as reaction gas.

The challenge with selenium speciation is the extraction of the organic species from the matrix. The protein-bound selenium species are usually extracted from the matrix using enzymes, but issues with recoveries and reproducibility have been reported. We have tested several methods for the extraction of selenium species from feed samples. The inorganic selenite and selenate usually show recoveries close to 100%. For selenomethionine, the most common organic selenium species, recoveries in reference materials using enzymatic extraction are about 80%. However, the type of matrix influences the enzymatic extraction, shown by highly variable recoveries of selenomethionine when mixing the reference material with different feed samples. The different extraction methods will be compared and challenges will be discussed.

(O-21)

A STUDY OF SELENOPROTEINS IN ATLANTIC SALMON (*SALMO SALAR*) USING HYPHENATED MASS SPECTROMETRY AND BIOINFORMATICS

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Selenium (Se) is an essential micronutrient for vertebrates and fish. Se is central to the function of selenoproteins, which play key roles in many biological functions including redox signaling, antioxidant defense, hormone metabolism, and immune responses. The number and expression levels of selenoproteins vary between different animal species with teleost fish featuring a much higher number of selenoproteins compared to vertebrates. While selenoproteomes have been well described for many species, a comprehensive analysis of selenoproteins in Atlantic salmon (*Salmo salar*) has yet to be performed. With recent advances in bioinformatics it has become possible to predict selenoproteins using computational tools; however, these in silico predictions description require validation through analytical data.

In the present study we applied gel electrophoresis with subsequent use of laser ablation coupled to inductively coupled plasma mass spectrometry (LA-ICP-MS), and tryptic digestion with subsequent analysis with high performance liquid chromatography (HPLC) coupled to both ICP-MS and high-resolution tandem electrospray mass spectrometry (HR-ESI-MS) for the analysis of selenooproteins. Furthermore, we set out to combine theoretical selenoprotein predictions with hyphenated analytical techniques to characterize the selenoproteome of salmon liver tissue. The results and challenges related to the analytical work will be presented and the presentation will show how bioinformatics data can be combined with analytical data to study selenoproteomes in fish.

(O-22)

BINDING OF ETHYLMERCURY FROM THIOMERSAL TO HEMAGGLUTININ IN INFLUENZA VACCINES

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Human exposure to mercury species can be traced back to diverse sources. In case of Ethylmercury (EtHg+), exposure is strictly anthropogenic and derived from the use of Thiomersal (THI) as preservative in multi-dose vials of vaccines. THI decomposes in aqueous media and the following release of EtHg+ leads to antimicrobial properties. Banned in the EU since 2001, multi-dose vials are still used in the USA and developing countries and contain approximately 25 µg Hg as EtHg+ per dose. The distribution pathways for EtHg+ in the human body are not fully understood and still under discussion. Adduct formation of EtHg+ with several blood proteins has already been investigated to contribute to the elucidation of EtHg+-toxicokinetics. For these investigations, it is necessary to conserve molecular information of mercury-protein adducts during analysis, while separation of protein adducts and non-bound Hg has to be achieved. Size discriminating techniques, like size exclusion chromatography (SEC), coupled to elemental detection, like inductively coupled plasma-mass spectrometry (ICP-MS), are particularly well suited for this purpose.

This study investigates the adduct formation of EtHg+ from THI with the active ingredient in influenza vaccines, hemagglutinin (HA), which is a membrane protein of virions. Experiments have been carried out using a single-dose vaccine, incubated with different concentrations of THI and adduct formation was investigated by ultrafiltration and subsequent total reflection x-ray fluorescence (TXRF) analysis in a qualitative manner. SEC/ICP-MS was applied to obtain further information on the size of the protein involved in adduct formation. Since non-bound EtHg+ adhered on the stationary phase of the SEC column and subsequent injections of thiol-containing compound showed false-positive results on the contaminated system, gradient elution using a complexing agent was developed. Using this approach, it was possible to show adduct formation of EtHg+ and HA. The use of a complexing agent allowed for quantification with THI and revealed that 0.56% of EtHg+ binds to HA in multi-dose influenza vaccines under the selected conditions.

(O-23)
PURITY DETERMINATION OF HIGH PURITY METALS – CONSIDERATIONS FROM A METROLOGY PERSPECTIVE

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Calibration standards are required by metrology institutes to provide calibration measurement services. They provide traceability to the International System of Units (SI) and are the basis of many calibration and measurement capability claims. High purity metals are the most common source for primary calibration standard preparation in inorganic analysis. Therefore, there is a need for metrology institutes worldwide to develop a sustainable strategy to assess the purity of these materials.

The work presented here will demonstrate the potential of inductively coupled plasma tandem mass spectrometry (ICP-MS/MS) as the centre piece, in combination with other techniques, for the determination of elemental impurities in high purity metals. Factors affecting the accuracy and uncertainty of the purity estimation by such techniques have been investigated. In particular, the measurement challenges posed by the matrix, the difficulty of combining impurity results from multiple techniques with different associated uncertainties (symmetrical with asymmetrical uncertainties), estimation of uncertainties obtained from small numbers of repeated determinations and on the basis of "expert judgment" still represent remaining challenges. Moreover, the effect of the purity value on the final uncertainty of the primary calibration standard mass fraction will be discussed. Finally, an overall strategy for impurity determination of high purity metals will be proposed.

(O-24)
METALLURGICAL ANALYSIS WITH ICP-OES: DEALING WITH THE MATRICES AND INTERFERENCES

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Metallurgical analysis can be a valuable source of information to any industry working with metals. Pure metals and alloys are produced at different grades/specifications depending on the end-use. It is important to accuatley measure the impurities as these may affect the performance and price of the final product. Due to the high concentration of certain analytes in the product, measuring the impurities in the metals can be challenging. When using ICP-OES many potential interfernences can cause your results to be biased.

This work presents the PerkinElmer Avio 500 ICP-OES to explore impurity analysis in metallurgical matrices, focusing on matrix tolerance and interferences. Pure lead and steel samples were analyzed for impurities. Multicompenent spectral fitting (MSF) was utilized to remove interfering spectral overlaps. Spike recoveries in a 1% Pb matrix resulted in an accuracy of 99.99% with stability of <5% variation over 6 hrs of continuous analysis. Steel samples were digested and analyzed without dilution at 1% dissolved solids and accuracy was demonstrated with quality controls and spike recoveries.

(O-25)

TRACE ANALYSIS OF EMERGING CONTAMINANTS IN RIVERINE, ESTUARINE AND COASTAL SYSTEMS USING ICP-MS/MS AND HYPHENATED TECHNIQUES

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Despite the ongoing reduction of emissions of contaminants into the environment, coastal zones still represent the most anthropogenically impacted ecosystems worldwide. In particular the ongoing evolution of coastal zones into industrialized areas e.g. due to extended shipping, oil and gas production, or offshore wind farms even boosted the direct release of either known, but also of various new contaminants into the marine environment.

To understand the interplay between such complex marine ecosystems and its main tributaries, sensitive and accurate new analytical approaches are needed to identify the sources, fate and behaviour of contaminants such as trace elements and their species within the environment. Even though many contaminants show only low concentrations in the environment they are of great concern due to their specific chemical properties and effects even at low dose, which makes highly sensitive analytical methods mandatory.

In particular recent developments in either multi element and isotopic analysis as well as within the field of speciation analysis of selected emerging contaminants opened new possibilities to conduct large scale environmental studies on the interactions of river catchments and coastal zones.

Especially the developments within the field of ICP-MS, which ends up in the recent introduction of ICP-MS-MS, strongly enhanced the possibilities in terms of accurate analysis of such complex samples.

This contribution will focus on the optimization and application of ICP-MS/MS for the analysis of Rare Earth Elements (REE) and selected species within the context of our current studies of different river catchments. In particular the application of the O2 mass shift mode offers new possibilities to overcome interference as well as sensitivity issues related with the analysis of the mentioned elements in complex environmental samples, which will be highlighted.

(O-26)

QUANTITATIVE METABOLITE PROFILING OF MEDICAL DRUGS VIA HIGH-PERFORMANCE LIQUID CHROMATOGRAPHY-INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY AFTER PRE-COLUMN DERIVATIZATION

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The development of suitable analytical methods for drug ADME (absorption, distribution, metabolism and excretion) studies is of great importance. Over the past decade, high-performance liquid chromatography-inductively coupled plasma mass spectrometry (HPLC-ICP-MS) has proven to be a promising technique for drug metabolite profiling. However, the wide and routine application of HPLC-ICP-MS in pharmaceutical R&D is seriously hindered by the fact that most of the drugs do not contain any ICP-MS detectable element. In this study, two cost-effective and commercially available derivatization reagents, tetrabromophthalic anhydride (TBPA) and p-bromophenacyl bromide (p-BPB), were selected for introducing an ICP-MS detectable hetero-element (Br) into amino group and carboxyl group containing pharmaceuticals and their metabolites, thus enabling the element-selective detection and quantification of these compounds, with a final aim of rendering HPLC-ICP-MS into a powerful technique for quantitative metabolite profiling in the pharmaceutical sciences. Levothyroxine and its metabolites (3,3´,5-triiodothyronine and 3,5-diiodothyronine) were used as amino group containing model compounds, diclofenac and its metabolite 4´-hydroxy-diclofenac were employed as carboxyl group containing model compounds. To ensure quantitative conversion of the target compounds in a realistic matrix (human plasma), the reaction conditions were carefully optimized. The derivatized sample was subjected to HPLC-ESI-MS for structure confirmation of the derivatives formed. In order to obtain a baseline separation of the derivatives from the interfering matrix components, the HPLC conditions were also optimized by investigating different chromatographic columns and eluent systems. Br containing derivatives were determined via ICP-MS(/MS) at a mass-to-charge ratio of 79 using H_2 as a reaction gas to ensure interference-free detection. Both of the methods were validated in accordance with the ICH Q2(R1) guideline by evaluating the selectivity, linearity, limit of quantification (LoQ), accuracy, and precision. The results showed that both of the methods demonstrate a fit-for-purpose accuracy (recovery between 85% and 115%) and precision (repeatability ≤15% RSD). In conclusion, the combination of chemical derivatization and HPLC-ICP-MS can overcome the typical absence of ICP-MS accessible elements in active pharmaceutical ingredients, thus enabling accurate quantification of specific metabolites in the absence of authentic standards, which can be used as a sterling alternative to radio-HPLC in some cases.

(O-27)

DETERMINATION OF TECHNOLOGICALLY CRITICAL ELEMENTS IN ENVIRONMENTAL AND CLINICAL SAMPLES BY ICP-MS

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The need to accurately measure concentrations of an ever broader range of elements in environmental and clinical samples is constantly growing. This interest stems from socio-economic factors, technological advances, environmental and public health concerns which increasingly focus on previously less studied, emerging contaminants such as technologically critical elements (TCE) presented in natural matrices at trace and ultra-trace levels. Global production of these low abundance elements has increased dramatically over the last few decades due to new emerging application areas, most notably in advanced electronics and the introduction of car catalysts worldwide.

State of the art inductively coupled plasma mass spectrometry (ICP-MS) instrumentation possesses the prerequisite sensitivity to carry out multi-elemental trace analyses at sub-ng l-1 to sub-pg l-1 levels in solution making the technique ideally suitable for TCE determination. Here we review ICP-SFMS (also known as HR-ICP-MS) figures of merit for multi-elemental trace analyses in environmental and clinical matrices.

(O-28)
IODINE IN SEAWEED - OCCURRENCE, SPECIATION, BIOAVAILABILITY AND RISK ASSESSMENT

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Seaweed is the common term for marine macroalgae plants, which may be divided into green, red and brown algae types. There is an increased interest to increase the exploitation of marine macroalgae for commercial purposes including the use in relation to food and feed production. Certain seaweeds have a great potential to accumulate various trace elements and contain consequently relatively high levels of both essential and toxic elements. Seaweed can even be used for bioremediation purposes in order to remove trace elements from the environment.

The concentrations of iodine in seaweeds vary highly between the different types of seaweed. In green and red algae concentrations in the lower mg/kg are typically reported, whereas in certain brown algae concentrations in the g/kg range (dry mass) can be found. These very high levels raise concern about food and feed safety when brown algae are used consumed by either humans or animals. No maximum levels for iodine in seaweeds (or other types of food and feed) have been established in the legislation in EU. For humans an upper tolerable level at 600 µg/day has been established (SCF, 2003), hence consumption of as low as 100 mg of certain seaweeds would lead to an exceeding of this guideline value.

There is a need for a better documentation of the iodine levels in seaweeds and further knowledge on the biological and environmental factors that may influence the concentration levels (e.g. seaweed type, location and season). Furthermore, the speciation of iodine may also be an important parameter to take into account when assessing the safety of seaweed food and feed applications.

The present lecture will include:
examples of the use of seaweeds in various food items examples of the determination of iodine and iodine compounds in seaweed samples by (HPLC-)ICP-MS discussion of the results obtained in relation to food and feed safety assessment.

(O-29)

MULTIMODAL ELEMENTAL AND MOLECULAR IMAGING ANALYSIS OF DRUGS ON ABUSE ON BLOTTER PAPERS

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Due to a present shortage of lysergic acid diethylamide (LSD), phenethylamine derivatives are sold as a replacement or deceptively as LSD itself. These potent and toxic substances can lead to severe intoxication, thus a more profound understanding of their biological effects is required. The manufacturing process of spraying these compounds onto the common blotter paper increases the risk of overdose due to heterogeneous distribution. Besides rapid detection of the analytes, the manufacturing process was elucidated via different imaging techniques. A sample, containing the two NBOMe derivatives iodophenethylamine (25I-NBOMe) and chlorophenethylamine (25C-NBOMe), was analyzed using imaging techniques such as micro x-ray fluorescence analysis (μXRF), laser ablation-(LA) inductively coupled plasma-optical emission spectroscopy (ICP-OES) and matrix assisted laser desorption ionization mass spectrometry (MALDI-MS). HPLC-MS/MS was used for validation purposes after extraction. Using the signal of chlorine and iodine from the compounds, μXRF proved to be the fastest, cheapest and easiest method for identification, requiring no sample preparation at all. LA-ICP-OES was used to obtain three-dimensional information of the compounds in the blotter paper. These results helped to confirm the assumption that manufacturers spray the compounds onto the paper. Whereas μXRF and LA-ICP-OES detected signals for chlorine and iodine, MALDI-imaging showed the molecular distribution of both analytes. HPLC-MS/MS measurements as a complementary method finally validated the results obtained by μXRF, LA-ICP-OES and MALDI-MS.

(O-30)

IDENTIFICATION AND QUANTIFICATION OF POTENTIALLY HAZARDOUS DECOMPOSITION PRODUCTS OF LITHIUM ION BATTERY ELECTROLYTES CHROMATOGRAPHIC TECHNIQUES WITH ICP-SF-MS DETECTION

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In present time, energy and more important energy storage are topics of utmost importance. With regard to the latter, the lithium ion battery (LIB) is one of the most promising candidates to fulfill the demanding requirements in terms of energy density, cycling stability and safety. But, state-of-the-art LIB electrolytes still show diverse decomposition mechanisms and consequently decomposition products that are yet to be understood. Therefore, quantitative data of the potential hazardousness of those compounds is crucial. This importance is even more emphasized since some decomposition products show structural similarities to phosphorus-based pesticides or even worse chemical warfare agents (CWAs).[1]

In this study both artificially aged electrolytes (high voltage, high temperature treatment) and field-tested automotive electrolytes were investigated in terms of identification and quantification of the PF_6^- decomposition route. [2]

Findings of the aged lab cells and field-tested cells are interrelated. For this, plasma-based techniques and organic mass spectrometers were used for complementary analysis in terms of quantification (of the phosphorus-containing species) and species identification. Since a large variety of compounds was found, comprehensive analysis using gas chromatography (volatile, non-acidic compounds) and hydrophilic interaction liquid chromatography (HILIC, non-volatile, acidic compounds) gave a complete overview of all species. The results are interpreted with regard to total decomposition products in electric vehicles; toxicological aspects are also taken into account.

[1] W. Weber, et al., *J. Chromatogr. A*, **2015**, *1394*, 128-136.
[2] V. Kraft, et al., *RSC Advances*, **2016**; 6, 8-17.

(O-31)

INVESTIGATION OF LITHIUM LOSSES IN LITHIUM ION BATTERIES BY MEANS OF PLASMA-BASED TECHNIQUES USING ISOTOPE LABELED MATERIALS

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Since the introduction of the lithium ion battery (LIB) in the early 90's, it has to face challenging demands for mobile and stationary applications, respectively. The negative electrodes of the state-of-the-art LIBs are based on carbonaceous material delivering a decent capacity of 372 mAh g^{-1}. Lithium transition metal oxides (LiMO_2; M = Mn, Co, Ni) are used as positive electrodes supplying capacities in the range of 150 mAh g^{-1} like ternary mixtures of nickel, cobalt and manganese (LiNi$_{1/3}$Co$_{1/3}$Mn$_{1/3}$O$_2$ (NCM111)). However, these materials suffer from fading capacities - especially at elevated charging cut-off voltages exceeding 4.4 V - which cause is still a matter of discussion in literature.[1,2]

One postulated degradation mechanism is assigned to the passivation layer on the carbonaceous negative electrode, which is called the solid electrolyte interphase (SEI). It is mainly formed during the first cycles due to the high reductive potential affecting the electrolyte and consuming active lithium (either from the conducting salt or the cathode material). Furthermore, the kinetic hindrance of lithium re-insertion into the transition metal oxide host structure is another debated mechanism.[1,2] In order to quantify the lithium loss in both positive and negative electrodes, plasma-based analytical techniques are well suited for these investigations.

In this work, inductively coupled plasma-optical emission spectroscopy (ICP-OES) is used to investigate the lithium loss in charge/discharge aged layered NCM-based cathode materials as well as the lithium loss in carbonaceous anodes using glow discharge-sector field-mass (GD-SF-MS). Additionally, investigations of ^{6}Li-isotope enriched cathode materials were conducted using inductively coupled plasma-mass spectrometry (ICP-MS) and GD-SF-MS for bulk and depth-resolved quantification of lithium losses in charge/discharge aged LIBs. Therefore, the NCM111 material is synthesized using ^{6}Li-enriched components as source material and cycled in a full-cell set-up to elucidate the origin of lithium losses. With this approach, it is possible to distinguish between losses either from the conducting salt or the cathode material.

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(O-32)
ANALYSIS OF NATURAL AND MANUFACTURED NANOPARTICLES IN COMPLEX SAMPLES

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The analysis of ENPs in consumer products and environmental compartments requires different approaches and has to answer fundamentally different questions. While in products it might be required to produce a quantitative particle size distribution of a known ingredient which is present in comparable high concentrations, analysis in the environment requires the identification of an ENP to be of industrial, manufactured origin often at very low concentrations. In products the analysis has to provide data compatible with existing or future definitions or regulations (e.g. number or mass-based particle size distributions) while in the natural environment it is of more interest which types of NPs are present and which of those are manufactured even though the exact type or composition of the ENPs are unknown. Depending on the type of ENPs and the chemistry of the matrix, methods could be extremely simple (Au-NPs in drinking water) or relatively complex (TiO_2 and Fe_3O_2 in sunscreen and TiO_2 in the environment). We have developed (validated) methods for cosmetics, food and soils/waters using specifically adapted sample preparation techniques and quantification with classical Field Flow Fractionation-ICPMS but also single particle techniques as ICP-TOFMS.

(O-33)

HOW ICP-MS CAN HELP TO STUDY THE FATE OF ENGINEERED NANOPARTICLES IN ENVIRONMENTAL MATRICES

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In this presentation, analytical methods based on inductively coupled plasma quadrupole mass spectrometry (ICP-MS) for ultra-trace detection of manufactured nanomaterials (MNMs) will be discussed and future trends will be outlined. Selected results from a European research project termed FENOMENO will be presented with a special focus on recent developments for direct, fast, and high-throughput nanomaterial characterization on a single particle level. FENOMENO is an integrative project aiming at an understanding of the impact of MNMs on the environment. Innovative analytical approaches are used to study the fate and effect of wastewater-borne MNMs in an aquatic ecosystem including analytical sensor systems, biochemical markers, and ICP-MS.

The benefits of stand-alone single-particle (sp) ICP-MS for the detection and characterization of single nanoparticles (NP) will be discussed. Instrumental modifications are not only helpful for total elemental analysis but also enable the detection, for example, of individual Ag, Au and TiO_2 nanoparticles with significantly improved size detection limits. The advantages and disadvantages of millisecond versus microsecond dwell times are critically discussed including potential measurement artifacts. A method for nanoparticle fractionation, size characterization, and quantification using capillary electrophoresis (CE) and ICP-MS as well as CE-SP-ICP-MS with dedicated online particle pre-concentration will be presented.

Because environmental concentrations of nanomaterials are at ultra trace levels, analytical methods often include sample preconcenctration and acidification of samples before sample storage. One major challenge for research in the coming decade is clearly the preservation of chemical things as they are in the orignal sample. Also, nanoparticle toxicity towards aquatic organism is typically tested using standardized test media but the nanoparticle fate in these media over the course of the toxicity test is not routinely checked. Here, SP-ICP-MS will be an important tool in the future that can provide information on effective concentration and nanoparticle size in toxicity assays.
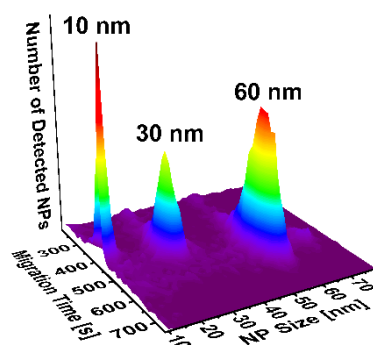

Figure 1: CE-ICP-MS electropherogram of a mixture of NIST AuNP reference materials.

(O-34)
FROM SINGLE PARTICLE TO SINGLE CELL ICP-MS: METHOD DEVELOPMENTS, ACHIEVEMENTS, AND CHALLENGES

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Since its introduction in 2012, ICP-MS/MS has gained great attention in elemental analysis. The ability to better control interference removal in the collision/reaction cell makes it quite superior to conventional single quadrupole instruments. Due to this, it might be also very promising for single particle (sp) and single cell ICP-MS (sc-ICP-MS), especially for challenging elements like Ti, P, Se, etc..

The first part of this presentation will highlight the use of triple quadrupole (TQ-)ICP-MS for the characterization of TiO_2 particles by sp-ICP-MS. Different measurement modes will be compared for their analytical figures of merit. This investigation showed that ^{48}Ti - as most abundant Ti isotope - measured in the TQ mode offered best analytical data, with either O_2 or NH_3 in the reaction cell. The monitored reaction products were at m/z 64 ($[^{48}Ti^{16}O]^+$) and 114 ($[^{48}Ti(^{14}N^1H_3)_3(^{14}N^1H)]^+$), resp., and were tested for the characterization of TiO_2 particles found in consumer products [1]. Important data like particle number concentration and particle size distribution are compared for different measurement modes.

Similar to sp-ICP-MS, single cell analysis is also accessible by ICP-MS. TQ-ICP-MS, for instance, makes possible the detection of constitutive elements like P (detected as $^{31}P^{16}O^+$) being useful as marker for cell detection. In this work, the combination of a microflow nebulizer (EnyaMist®) with a total consumption spray chamber was tested for this purpose [2]. Under optimized conditions, achievable transport efficiency was up to 25 %. The analysis of different selenized yeast samples demonstrated that the type of incorporation are easily distinguishable by sc-TQ-ICP-MS. Moreover, quantitative data on the number of cells with incorporated Se are available.

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(O-35)

CHARACTERIZATION OF NANOPARTICLES IN FOOD USING ICP-MS – HOW FAR HAVE WE COME IN THE LAST 10 YEARS?

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Nanotechnology and more particularly nanotechnology-based products and materials have a large potential for providing novel solutions to many of the current challenges facing society such as energy supply and resources efficiency, a clean environment, information and communication, mobility and security, and the efficiency of health-related products. Current applications in the agri/feed/food sector are food additives and food contact materials, whereas potential future developments are expected in the field of nanoencapsulates and nanocomposites in applications such as novel foods, food/feed additives, biocides, pesticides and food contact materials. With the increasing use of nanotechnology, there is a need for reliable detection and characterization methods for nanoparticles (NPs) in food and biological matrices. For regulatory purposes (e.g. Novel food, "Food labelling"), the European Commission developed a recommendation for the definition of a nanomaterial, which poses additional analytical challenges such as the need for determining a number-based particle size distribution.

This talk will present examples of analytical challenges and solutions based on DTU Food's work with nanoparticles throughout the last 10 years. We did our first steps into the "nanoworld" by establishing an analytical platform for analysis of gold NPs based on asymmetric flow field-flow fractionation (AF4) coupled online with light scattering detection and inductively coupled plasma-mass spectrometry (ICP-MS). Thereafter, we performed oral exposure studies with silver and selenium NPs in rats and we were challenged with the question of where to find the "needle in the haystack". With direct focus on methods for NPs in food in the EU project "NanoLyse", we developed and validated a method for silver NPs in chicken meat based on AF4-ICP-MS. Since a few years, single particle ICP-MS has become increasingly popular and we applied the technique for several applications including chicken meat (silver NPs), game meet (lead NPs), food simulants (silver NPs), candy (titanium dioxide NPs) and noodles (aluminum-containing NPs). In our experience, single particle ICP-MS is a powerful screening method for the presence of NPs, but an accurate and precise determination of particle size distribution and concentration is hardly ever possible. Currently, we are working on the development of screening procedures for NPs in food and methods for polymeric NPs ("nanoplastics").

Throughout our work, we identified sample preparation as the most critical step of the method. NPs often interact with each other or with their surroundings leading e.g. to aggregation, adhesion to surfaces or dissolution. In general, a combination of several techniques is required for successful analysis of NPs in food and biological samples and suitable reference materials for method validation are lacking. Accurate and precise characterization of metrics such as size, shape, particle mass and number concentration therefore remains a challenging analytical task.

(O-36)

THE USE OF SINGLE PARTICLE INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY TOWARDS ANSWERING REAL WORLD QUESTIONS IN THE ENERGY AND CHEMICAL INDUSTRY

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In this study, we used single particle inductively coupled plasma mass spectrometry (spICP-MS) to answer nanoparticle size questions in real world energy and chemical samples that traditionally use TEM, SEM, NTA for size characterization. We will cover 2 separate sample types.

In the first example, the presence of heteroatoms in MFI nanoparticle solutions were explored. This new sp-ICP-MS method gives the unique ability to monitor heteratom incorporation into zeolite particles as a function of reaction time. Multiple samples were taken over various time points of the zeolite synthesis and were analyzed by this technique. The results showed different uptake into the MFI-zeolite crystal for the various heteratoms of interest (Al, Fe, W of interest). In this presentation, we report nanoparticle concentrations and particle size distributions for all zeolite samples. This study demonstrates the applicability of spICP-MS to characterize heteroatoms, and compares the results with other characterization techniques.

In the second example we used spICP-MS/MS for the particle size determination of ultradispersed-catalysts in bitumen or heavy oil fractions. Here, we present the application of this technique using a tri-metallic ultradispersed catalyst formulation containing Mo, Ni, W dispersed in vacuum residue, which was selected to determine the best conditions to run sp-ICP-MS/MS in hydrocarbon media by using a commercially available ICP-MS/MS instrument. Plasma stability in hydrocarbon media, nebulization efficiency and interference removal were evaluated. Results obtained by sp-ICP-MS/MS were compared to nanoparticle tracking analysis (NTA) results on such samples, using the methodology reported elsewhere very recently.

(O-37)
SINGLE CELL ICP-MS: THE ADVANTAGES OF QUATIFYING THE METAL CONTENT IN INDIVIDUAL CELLS

Chady Stephan, David Price and Ruth Merrifield

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The ability to rapidly quantify the elemental concentration of individual cells, as well as the distribution in concentration throughout the cell population, has been a limiting factor in life science applications that focus on uptake rates, bioavailability, and bioaccumulation for drug delivery and toxicity assessment. Traditional methods for measuring uptake rates can be a time-consuming process with long instrument analysis and sample preparation times, often leading to qualitative or population-averaged results. We present a new technique, Single Cell ICP-MS (SC-ICP-MS), which is capable of overcoming this and offers a unique opportunity to quantitatively measure the metal content in individual cells, unveiling new capabilities to study intrinsic metals and the uptake of dissolved (ionic) and nanoparticulate metals into cells. This novel approach provides new insights into drug delivery, toxicity assessment, bioavailability and bioaccumulation mechanisms. Here we will share insights into the uptake of cisplatin into ovarian cancer lines as well as nanoparticles into algal cells to show the power of this technique for the development of targeted drugs and the toxicity of metals to environmental systems, giving fast and in-depth information on the mass and distribution mass of metals in cells that can be linked to biological cellular responses.

(O-38)

INNOVATIONS IN SINGLE PARTICLE ICP-MS – ACCURATE DETECTION OF PURE AND ALLOYED NANOPARTICLES

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Since the release of SP-ICP-MS by PerkinElmer in 2014 it has become a staple analysis tool for particle counting and sizing in the nanoparticle (NP) world. It is now widely accepted as a technique for NP analysis in a wide variety of industries from environmental, food, semi-con and health sciences with a standardized method released by ISO (19590:2017) and another coming from ASTM (WK55613) in the near future. Although the technique is now seen as a standard method, the technology, applications and analysis techniques are still rapidly advancing. Here we would like to talk about recent advances in SP-ICP-MS to include: quantifiable dual analyte analysis enabling particle source identification, clustering techniques enabling enhanced particle size detection and the use of All Matrix Solution (AMS) inline dilution to prevent NP transformations from sample preparation.

(O-39)

STUDY OF THE ION CLOUD FORMATION FROM GOLD NANOPARTICLES IN ICP-MS BY MEANS OF MICROSECOND DWELL TIME SP-ICP-MS

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As the number of nanoparticle applications in technology, medicine, and consumer products increases, there is also a growing interest in the characterization of nanoparticles (NP), engineered as well as naturally occurring. Commonly used engineered inorganic particles are made of gold and silver, which can be found in biosensor applications, cancer treatment, or disinfection. To optimize those applications and deal with risk assessment, the particles' most important characteristics like number concentration, particle size distribution, and elemental composition need to be determined – at best by a fast and versatile method.

Single particle-inductively coupled plasma-mass spectrometry (sp-ICP-MS) has emerged as a powerful analytical technique to determine size distributions of nanoparticles as well as their number concentrations. It offers unique capabilities compared to other established characterization methods – such as UV/vis-absorption spectroscopy, light scattering or electron microscopy. For further development of the technique, fundamental characteristics of the formed ion clouds from introduced NP into the ICP need to be studied. This is achieved by fast data acquisition rates in the microsecond range and extensive data evaluation.

In this study, we focus on the influence of the particle diameter on the extension of the formed ion clouds by introducing precisely sized gold nanoparticles from 15 to 100 nm in sp-ICP-MS. This allows to discuss critical method parameters in sp-ICP-MS for number concentration and size determination.
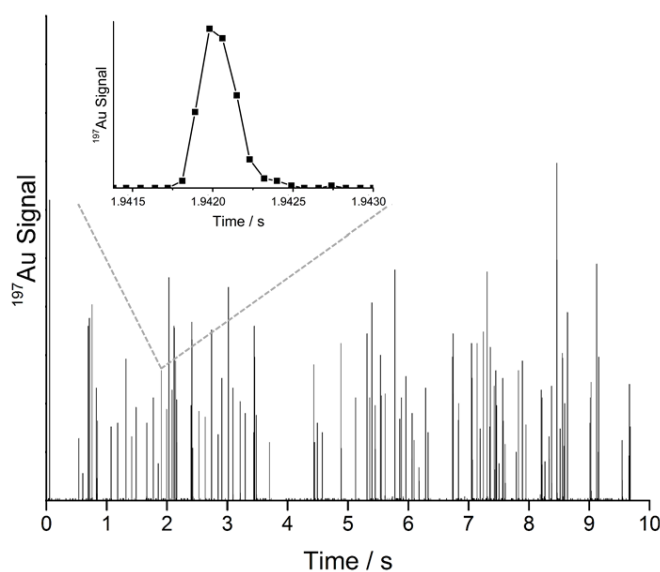

Figure 1: Time resolved ^{197}Au-signal recorded by introducing AuNPs under single particle conditions. Enlarged section shows the profile of one exemplary picked single particle event.

(O-40)

EXPLORATION OF BRAIN IRON BALANCE USING STABLE ISOTOPE TECHNIQUES

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Iron is an essential nutrient for all forms of terrestrial life and is vital for normal organ and cellular function, including the human brain. However, even traces of ferrous iron can be highly toxic to the body by catalysing the formation of highly reactive oxygen species (ROS). Iron induced oxidative stress has been associated with the development of diabetes type 2 and cardiovascular disease. Remarkably, brain iron accumulation is also a common feature of neurodegenerative disorders.

Brain iron influx is thought to be marginal in healthy adults once brain development is complete. This raises the question if brain iron accumulation occurs only in states of disease or if brain iron uptake in adulthood is higher than commonly assumed due to methodological limitation of radiotracer techniques as employed in previous studies.

Recently, we have pioneered novel concepts for tracing brain iron influx and assess brain iron balance in rats and mice to study brain iron homeostasis *in vivo* using stable isotope tracers. Up to three tracers (^{54}Fe, ^{57}Fe and ^{58}Fe) were fed continuously up to 4 months in intervals to quantify brain iron transfer from feed to brain and its export from brain.

By overcoming limitations of radiotracer techniques, we could confirm that absolute brain iron uptake from feed in adulthood is minute but could also uncover that relative brain iron uptake is significant even in the healthy organism. Common radiotracer protocols permit to study tracer fluxes but not fluxes of natural iron in and out of brain as our novel methodology.

Iron uptake was found to exceed iron efflux which points to iron accumulation to occur in the mammalian brain over life-time even under non-pathological conditions. Subsequent intervention studies targeting diet showed for the first time that brain iron influx is dependent on dietary iron intake despite the rather small fraction of whole body iron present in brain. Intestinal iron absorption was also found to determine brain iron influx when the feed was supplemented with zinc. Zinc is known to compete with iron for intestinal uptake and to suppress iron absorption.

Imaging of elemental and tracer distribution in brain slices by LA-ICP-MS at the University of Tokyo shows that iron concentration is the highest in the hippocampus and substantia nigra as areas affected strongly in Alzheimer's and Parkinson's disease. Exchange of natural iron by tracer iron was found to be slower in these regions than in other regions of the brain. This indicates either that iron turnover in these regions is slow or some iron is resistant to turnover as given for brain iron deposits.

Taken together, our observations point to a possible role of iron nutrition in brain iron accumulation on from young age and, thus, a nutritional component in the development of neurodegenerative disorders.

(O-41)
ON-LINE STEEL SLAG ANALYSIS WITH LIBS – A CHALLENGE AND AN OPPORTUNITY

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Slag is produced in very large quantities in steel production. The chemical composition of the slag is very important for the steel quality, and therefore of interest to monitor closely in the steel process. The slag is also a product, widely used in e.g. road construction, concrete and as raw material in the production of insulation ("Rockwool"). The challenge is to develop a fast method for chemical analysis of slag and similar rest products, applicable in-situ without sample preparation. Such a method is needed for improved process control, as well as increased reuse of slag in a circular economy.

Currently, the most common method for slag analysis is X-ray fluorescence (XRF). This technique has outstanding analytical precision, but requires more or less time-consuming sample preparation. The slag is ground to a fine powder, homogenised and pressed into a pellet or fused with e.g. lithium borate to a glass bead. A technique with the potential for considerably faster analytical response is Laser Induced Breakdown Spectroscopy (LIBS). Due to the stand-off capability of LIBS, it is even feasible to analyse hot slag directly above the steel converter, as already demonstrated by Sturm et.al. [1].

One of the major challenges in slag analysis is the inhomogeneity, detrimental to both accuracy and precision. Since the aim is to reduce total analysis time, sample preparation must be kept to a minimum. In this work, we have used slag samples coarsely crushed to large grains of cm to mm size. The LIBS system is based on a YAG laser with 200 mJ focused at   1 m from the sample, and two Avantes miniature spectrometers as detectors. A simple sample holder was designed in the form of a small cup with both rotational and translational movement. In this way, a relatively large area approximately one cm^2 can be sampled by a few hundred laser shots, distributed over a considerably larger area including several grains. A large number of slags of different types have been analysed with this technique, both in the laboratory and in field tests "on the factory floor" in steel works. The LIBS system was calibrated using slag samples analysed with XRF with good results. Precision tests on a few slag samples were compared with XRF data, showing very similar results. The relative standard deviations (RSD) for major elements were typically in the range 1 – 3%, which is very satisfactory. The experimental details and results of the work will be presented, and the prospects for further development will be discussed.

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(O-42)

INVESTIGATION OF EXTREME NATURAL ABUNDANCE VARIATION OF MULTIPLE ISOTOPIC SYSTEMS (B, ZN, SR, MO, ND AND PB) IN THE NORTH SEA ESTUARY

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Isotopic signatures can serve to trace and understand pollution dynamics and the discharge characteristics of riverine inputs into coastal seas, usually representing complex, highly dynamic and anthropogenically impacted aquatic ecosystems. Different marine and estuarine compartments (sampled between 2014 and 2017), covering the catchment of the German Wadden Sea and its main tributaries, the Elbe, Weser, Ems and Rhine River, were investigated by multi collector inductively coupled plasma mass spectrometry (MC ICP-MS).

The determination of the isotopic variations of B, Zn, Sr, Mo, Nd and Pb in different marine and riverine compartments highlights the potential of this unique multi-isotopic approach. The characteristics of the Elbe River is described by using physicochemical maps and aquatic isoscapes to study aquatic ecosystem mixing and transport processes. Aquatic isoscapes were created using ArcGIS® by relating spatial elemental and isotopic data with geographical and geological maps. These maps show large variation for different parameters and also reflect the numerous impact factors (e.g. geology, anthropogenic sources) influencing the catchment area. Large natural abundance variations of all investigated isotopic systems were observed within a small observation area. For example, the Elbe catchment shows characteristic mixing occurrences between freshwater and seawater signatures of $\delta(^{11}B/^{10}B)_{SRM951a}$ ranging from (-5.47) to (+37.89), $n(^{87}Sr)/n(^{86}Sr)$ ranging from 0.70667 to 0.71374, $\delta(^{66}Zn/^{64}Zn)_{IRMM3702}$ ranging from (-0.51) to (+1.17) and $\delta(^{98}Mo/^{95}Mo)_{SRM3431}$ ranging from (+0.63) to (+2.23) in the water body. The investigated area is especially characterized by extreme hot-spots showing highly radiogenic Pb isotope ratios $n(^{208}Pb)/n(^{204}Pb)$ ranging between 38.2 and 73.9 in the surface sediment. These Pb isotope ratios are among the highest reported values for terrestrial materials and indicate human impact by deposition of industrial waste.

(O-43)

DOUBLE PULSE LASER ABLATION IONIZATION MASS SPECTROMETRY

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Ultrashort-pulsed laser ablation and ionization sources allowed to improve significantly the measurement performance and capabilities of laser ablation based measurement techniques, including e.g. improved ionization efficiencies and plasma stoichiometry, clean and spatially more confined material removal, among others. However, and as discussed in various studies, clusters and molecules are observed to be formed in the plasmas, which might influence the analytical capabilities of the measurement system used if they mask an element of interest. In comparison to e.g. ablation plasmas induced by nanosecond pulsed laser systems the temperature of plasmas generated by femtosecond pulsed lasers are observed to be colder which favors the observed formation of such species [1].

In this contribution, the impact of a double pulse femtosecond laser ablation ionization source (first pulse for material ablation, second for plasma heating) on cluster formation and plasma stoichiometry will be discussed [2]. For performance evaluation systematic parametric studies (delay between both pulses, pulse energy) were conducted on various samples, including a high purity magnesium sample used as case study and different certified reference materials from NIST (SRM 661, 664, and 665). The measurements were finally compared with measurements conducted using a single pulsed measurement scheme. At optimal measurement conditions, a significant increase of singly charged element/isotopes and at the same time a reduction of detected clusters and molecules were observed, which enhance the qualitative and quantitative analytical capabilities of the LIMS system used in this study.

The measurements were conducted using our miniature (Ø60 mm x 160 mm) reflectrontype time-of-flight laser ablation and ionization mass spectrometer designed originally for the analysis of the chemical composition (elements and isotopes) of solids on planetary surfaces [3]. For ablation and ionization of sample material a femtosecond laser system is used, operated at a wavelength of 775 nm, pulse repetition rate of 1 kHz, and pulse energy $\leq$ 1 mJ [4]. For the realization of the double pulse measurement scheme, a beam splitter and a retro reflector positioned on a remotely controllable delay stage (length of 100 mm, delays of -300 to $+300$ ps can be achieved) are integrated in the current beam delivery system. The energy of the first and second laser pulse can be controlled independently, by changing the output power of the laser system and using an additional polarization attenuator, respectively [2]. The current beam guiding system will be discussed in more detail during the contribution.

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(O-44)

CHALLENGES AND STRATEGIES IN LA-ICP-MS - FROM BULK ANALYSIS TO IMAGING (AND BEYOND)

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Since the inception of the technique in eighties, laser-ablation ICP-MS has become a well-established microanalytical technique and has found its way into many labs around the world, either for fundamental studies or for purely applicative work. Most commercial systems usually comprise of a nanosecond solid state or excimer LA unit interfaced with a quadrupole ICP-MS. These systems are routinely used for research and applicative work, while femtosecond LA units and hi-resolution ICP-MS instruments - and also recently time-of-flight-ICP-MS - seem to be reserved mostly for fundamental research and geochemical and isotope analyses.

From the practical point of view users would usually quickly like to progress from relatively easy single point or line-scanning analyses for screening purposes towards advanced and fully quantitative 2D or even 3D LA-ICP-MS imaging and start solving interesting applicative problems. While this seems logical and quite straightforward, many aspects have to be adequately addressed for it to be successful. The challenges and strategies in working with LA-ICP-MS technique (ns-LA and Q-MS) at the National Institute of Chemistry, Ljubljana, Slovenia, since we started in this research field some 12 years ago will be discussed. These include calibration for bulk and imaging work, fabrication of standards for bio-imaging, use of glass standards for investigations of glass corrosion phenomena and ceramic glazes (quantitative surface and pseudo-cross-section analyses), etc. Modelling approaches and strategies for imaging will be discussed, with emphasis on understanding the resolution, noise, contrast and quality of LA-ICP-MS elemental images, all critically linked to instrumental parameters and sample properties.

(O-45)

ADVANCES IN TRIPLE QUADRUPOLE ICP-MS FOR ENVIRONMENTAL AND FOOD ANALYSIS.

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Following its commercial introduction in the 1980's, ICP-MS revolutionised trace elemental analysis by providing fast, multi-element detection for a wide range of applications. Early in its development, however, polyatomic interferences derived from combination of the sample components and the plasma gas were found to limit the performance of the instrumentation. Furthermore, it was observed that isobaric overlap from isotopes of other elements having the same mass as the element of interest also caused significant interference. Development of collision cell technology for interference removal provided a major improvement, but even this innovation couldn't fully remove every polyatomic interference or solve the problem of isobaric interferences.

Nevertheless, today ICP-MS is routinely used for analysis of trace elements in a wide variety of matrices, including environmental samples, such as waters and soils, all kinds of food and consumer products, clinical research specimens, advanced materials and geological, nuclear and semiconductor samples.

With the advent of triple quadrupole ICP-MS, a new level of interference removal has been achieved. The implementation of an additional quadrupole before the collision cell of the instrument allows pre-filtering of the ion beam to selectively transmit only the masses of interest, which alleviates the problem of unwanted side interference production in the cell through collisions between other masses in the sample and the cell gas. This pre-filtering capability also allows selective chemical reactions to be conducted in the cell to enhance polyatomic interference removal and, in many cases, solve the problem of isobaric overlap.

Although triple quadrupole ICP-MS is widely recognized as a major step forward for trace elemental analysis, it is not yet generally accepted as an alternative to collision cell based single quadrupole ICP-MS for routine applications. In this presentation, the latest advances in triple quadrupole ICP-MS technology and how these apply to routine analysis will be described. The enhanced performance provided by this technique will also be discussed, with a particular focus on its applicability in routine analysis of environmental and food samples.

(O-46)
CONTRIBUTION FROM LONG-RANGE TRANSPORT TO ELEMENT DISTRIBUTION IN NATURAL SURFACE SOILS: EXAMPLES FROM NORWAY USING ICPMS

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Sector-field ICP-MS facilitates the determination of around 60 elements in acid extracts of soil samples. A natural surface soil in Norway typically has a surface layer consisting mainly of humic material acting as an efficient filter for substances supplied by atmospheric deposition, including pollutants from long-range atmospheric transport. In this presentation data from extensive soil surveys will be discussed with respect to natural and anthropogenic sources, with emphasis on contributions from long-range atmospheric transport. A novel aspect of this work is the ratios of plutonium isotopes (^{239}Pu and ^{240}Pu) to distinguish between contributions from atmospheric nuclear weapons testing and the Chernobyl reactor accident.

(O-47)

APPLICATIONS OF ISOTOPIC MEASUREMENTS FOR DETERMINATION OF LONG LIVED RADIONUCLIDES IN THE OPEN OCEAN

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Nuclear and isotopic techniques are currently providing a unique source of information for identifying long lived radionuclides and tracing their pathways in the environment and, potentially, for investigating their biological effects on marine organisms. They provide tools also to investigate sea resources, oceanographic processes and marine contamination on a quantitative basis and at the same time address the problems of coastal zone management. The identification of sources of environmental contamination can be done by an isotopic abundance and/or an isotopic ratio analysis. Once the different sources are identified, the isotopic abundances and the isotopic ratios can be used to quantify the contribution of each source by source apportionment. Isotopic signatures are the basis for investigation of historical and environmental changes of the examined sampling sites.

Accurate analytical methodologies for plutonium, uranium and thorium in sea water based on the application of High Resolution ICP-MS in parallel with solid metrological concepts (uncertainty, traceability and validation) were developed in this study.

Several methods for sample preparation, separation and preconcentration of the analytes of interest, based on solid-phase extraction (SPE) with chelate resins were investigated and applied. High resolution mode of ICP-MS measurements was used for quantitative determination of plutonium, uranium, thorium in the open ocean and alternatively as a tool for studies on the isotopic fractionations during the sample preparation process isotopic ratio analysis. Isotopic signatures were used for investigation of environmental changes in several sampling sites.
Obtained in this study results represent an important step in the identification and enhancement of our understanding of the pollution sources in the open ocean.

(O-48)

ANALYSIS OF URANIUM USING OFF-LINE AND IN-LINE AUTOMATED SAMPLE PREPARATION TECHNIQUES FOR ICP-OES

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The determination of trace elements in uranium (U) and/or plutonium (Pu) materials are an important step for several areas including nuclear energy, forensics, space exploration, and military applications. The most common method for the detection of trace elements is by ICP-OES and/or ICP-MS. For this work, ICP-OES is employed due to its smaller footprint, ability to be housed completely inside a glove box, and ability to analyze for elements that may be difficult by ICP-MS such as Ca, K, Na, Mg, and Fe. However, in order to analyze trace elements in the presence of uranium, the emission rich uranium matrix must be removed. The removal of the U matrix has been achieved using Eichrome's UTEVA resin by manual gravity fed chromatographic separations. Recently, we have automated the off-line sample preparation process using the prepFAST MC from Elemental Scientific, Inc. (ESI) which has reduced the time, sample volume, and reagents volume. For some samples all of the work needs to be housed in a glove box for health and safety reasons, thus we have developed an in-line separation method using ESI's prepFAST IC for separating the trace elements from the uranium matrix. This in-line method further reduces the sample volume needed (67 µL of sample) and time required to get results (takes < 10 minutes per sample). In addition, the prepFAST IC utilizes the ability to do in-line dilutions which automates the calibration of the instrument. Furthermore, any samples that are outside of the calibration curve can be automatically diluted in-line to a factor that will be within the curve, reducing the user interaction with potentially harmful samples. The following work will present the accuracy and precision, as well as the method details for the prepFAST MC and prepFAST IC separation techniques.

(O-49)

DETERMINATION OF ^{236}U/^{238}U RATIOS IN ENVIRONMENTAL SAMPLES USING ICP-MS/MS

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On account of the virtual absence of ^{236}U in the environment and its abundance closely related to its provenance, the ^{236}U/^{238}U ratio has been commonly employed as a tracer to provide information on source identification for safeguard purposes, nuclear forensic studies and environmental monitoring.

Due to their high performance capabilities, ICP-MS techniques are currently the most widely employed to perform radionuclide determination. However, in the case of ^{236}U and due to its very low relative abundance, its determination is limited by the formation of ^{235}U^{1}H^{+} in the plasma and by the influence of the tail of the major isotope ^{238}U (abundance sensitivity).

In this work, we present an approach based on the ICP-MS/MS technology to determine ^{236}U/^{238}U ratios in environmental samples. The combination of two quadrupole-based mass filters, before (Q1) and after (Q2) the cell, in the MS/MS configuration provides abundance sensitivity values lower than 10^{-10}, avoiding the influence of the ^{238}U tail. In order to reduce the influence of the hydride–based interferences, different desolvation systems have been evaluated in relation to the sensitivity and the uranium hydride rate. In-cell ion-molecule reactions with O_2 and CO_2 have also been assessed to detect the uranium isotopes in mass-shift mode (Q1: U^{+} $\rightarrow$ Q2: UO^{+}). Best conditions provided a hydride rate value (^{235}U^{16}O^{1}H^{+}/^{235}U^{16}O^{+}) in the order of 10^{-7}. Finally, the methodology was validated with IRMM certified standards, and successfully applied to the determination of ^{236}U/^{238}U ratios in environmental samples corresponding to sediments originating from the radioactive contamination plume caused by the Fukushima Daiichi Nuclear Power Plant accident. Ratios down to 10^{-9} have been obtained with precisions lower than 20%.

13   Short Course Abstracts

(A-1)
FUNDAMENTALS OF LASER OPERATION

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Lasers are widely used in plasma spectrochemistry and serve as vehicles for sampling (e.g., laser ablation), plasma generation (e.g. Laser-Induced Breakdown Spectroscopy or LIBS), electronic excitation (e.g., laser-induced fluorescence) and plasma diagnostics (e.g., Thomson scattering, Raman spectroscopy, fluorescence-based mapping). In addition, lasers are finding use in relatively new areas such as Laser-Ablation Molecular Isotope Spectroscopy (LAMIS) and plasma-filament generation. Yet, despite this widespread utilization and broad application, many laser users are relatively unfamiliar with how lasers work and the many different kinds of lasers that exist. This short course will begin with a tutorial on laser basics and will cover a range of laser characteristics and how they arise. Included will be continuous-wave (CW) lasers, giant-pulse lasers, short-pulse lasers, narrow-band lasers, and tunable lasers.

(A-2)

IUPAC COMMISSION ON ISOTOPIC ABUNDANCES AND ATOMIC WEIGHTS (CIAAW): TABLES OF ISOTOPIC COMPOSITION OF THE ELEMENTS AND STANDARD ATOMIC WEIGHTS AND THEIR RELEVANCE FOR THE PLASMA SPECTROCHEMIST

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The Commission on Isotopic Abundances and Atomic Weights (CIAAW) is an international scientific committee of the International Union of Pure and Applied Chemistry (IUPAC) under its Inorganic Chemistry Division and entrusted with periodic critical evaluation of atomic weights of elements.

Formally established in 1899, the Commission on Isotopic Abundances and Atomic Weights remains one of the oldest continuously serving scientific bodies. It was created in order to introduce uniformity in the atomic-weight values used worldwide. Since 1970s, CIAAW evaluates in addition other cognate data, such as the isotopic composition of elements. Members of the Commission meet biennially where matters pertaining to the Commission's purview are discussed. The biennial CIAAW Standard Atomic Weights serve as primary source for Atomic Weight values worldwide for science, trade and education. The tables serve as the authoritative source and appear worldwide on the periodic table charts. Several subcommittees of CIAAW are entrusted with related topics such as e.g. isotopic abundance measurements, stable isotope reference material assessment and the natural assessment of fundamental understanding of isotopes.

Besides the Table of Isotopic Composition of Elements (TICE) and the Table of Standard Atomic Weights (TSAW), the Commission publishes a variety of relevant documents: Atomic Weight reports, isotopic composition reports, element-by-element reviews and technical and educational publications (e.g. assessment of reference materials for isotope values). All documents are also available on the CIAAW webpage (www.ciaaw.org) along with further information about commission-related topics and useful tools (e.g. the molecular-weight-calculator).

This short course gives an introduction to the Commission, its key tasks and functions as well as current projects relevant to the mass spectrometric community. Practical considerations for the plasma spectrochemist are provided concerning (1) the appropriate / inappropriate use of the CIAAW publications and the tabulated atomic-weight and isotope-abundance values; (2) the importance of correct and transparent extraction and application of these values and recommendations and in analytical chemistry; (3) isotope-abundance measurements and certified reference materials and (4) the importance of measurement uncertainty along with a guide on how to calculate and extract uncertainties from tabulated values. Recommendations will be discussed interactively on examples taken from daily lab routine.

Participants are asked to bring their own laptop computers.

(A-3)
PRACTICAL APPROCACHES TO USE REACTION GASES IN ICP-QQQ-MS

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This short course will show how to proceed in method development working with an ICP-MS triple quadrupole. The course is aimed at users of ICP-QQQ who would like to get more knowledge about the reactions in the reaction cell and how to change these reactions. The following questions will be addressed:

How can the reaction enthalpy be calculated?
Does the interference or the analyte have an exothermic or endothermic reaction with the added gas?
How does the collision energy affect the reactions in the cell?
Why is the ionization energy important?
Which gases are suitable for the different analytes and mass interferences? What are the products?
Regarding manually optimizing of the cell parameters, which parameters are important? How do these affect the reaction efficiency?

These questions will be answered with examples on polyatomic-, doubly charged-, and isobar mass interferences.

(A-4)
TIME-OF-FLIGHT MASS SPECTROMETRY FOR ATOMIC ANALYSIS

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Time-of-flight mass spectrometry (TOFMS) is among the simplest of mass analyzers, but it has demonstrated extensive analytical utility and significant potential for elemental analysis. TOFMS offers simultaneous multielement analysis at exceptionally high spectral generation rates (typically 20,000 complete mass spectra per second), adequate mass spectral resolving power (1500), high abundance sensitivity, the promise of high ion transmission efficiency at relatively low cost. Moreover, since each packet of ions is sampled from the sampled from the primary ion beam at the same instant, ion signals can be ratioed to improve precision for all isotopes and elements simultaneously the spectral skew that limit sequentially-scanned mass analyzers avoided. On the whole, TOFMS is an ideal mass spectrometer for transient analyses. In this short course, the fundamentals of TOFMS for use in atomic spectrometry will be reviewed, and instrumental and experimental considerations discussed. Applications of TOFMS with plasma ionization sources will be examined, and particular attention will be given to methods that exploit the characteristics of TOFMS to overcome typical experimental difficulties. Finally, approaches to improve TOFMS performance in future generations of instrumentation will be examined.

(B-1)
COMPLEMENTARY ELEMENTAL AND MOLECULAR BIOIMAGING TECHNIQUES: INSTRUMENTATION, METHODS AND APPLICATIONS

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Imaging methods have become apparent as important tools in many application areas of the Metallomics field, including studies on the distribution and the effects of (metallo)pharmaceuticals in the body, on the role of nutrients in plants, animals and humans and on toxic effects of compounds and nanoparticles. To further improve the information gained from imaging experiments, the combination of complementary imaging techniques to solve complex questions has strongly increased in recent years. Combinations of chemical imaging methods including MALDI-MS, µXRF or LA-ICP-MS or of chemical *in vitro* methods with medical *in vivo* imaging methods including CT or MRI provide valuable additional information.

Within this short course, strategies and examples for the combined use of several chemical and medical imaging techniques are presented, with a particular focus on complementary methods to LA-ICP-MS. These include the analysis of iodine and gadolinium containing CT and MRI contrast agents in human and animal tissue samples. Requirements for sample preparation and quantification will be discussed as well as possibilities and remaining challenges in this field. While the medical imaging techniques allow a 3-dimensional *in vivo* analysis, the rich chemical information particularly when using molecular and elemental mass spectrometry, the possibility for unambiguous quantification and a superior lateral resolution are advantages of the chemical methods.

(B-2)
A GUIDE TO METHOD DEVELOPMENT FOR FIELD FLOW FRACTIONATION ANALYSIS OF NATURAL AND MANUFACTURED NANOPARTICLES

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Field Flow Fractionation (FFF) analysis is a powerful tool to separate and size nanoparticles and coupled to ICPMS it can provide a speciation analysis of particulates in the size range of 1 to 1000 nm. However, we have to accept that the particle separation process in FFF is essentially different to the processes in gas and liquid chromatography. In principle it is a neat kind of colloid chemistry performed in a dynamic flow environment and in the vicinity of a wall. While the theory of FFF separations is very well developed, the practical application in many laboratories is hindered by unexpected, non-ideal behavior of many samples during the separation process.

This course shall provide first-hand experience and advice for FFF method development from the perspective of more than 20 years of, regrettably not always successful, FFF work.

(B-3)
SOURCES OF CONTAMINATION AND REMEDIAL STRATEGIES

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In theory, state of the art inductively coupled plasma mass spectrometry (ICP-MS) instrumentation possesses the prerequisite sensitivity to carry out multi-elemental trace analyses at sub-ng l^{-1} to sub-pg l^{-1} levels in solution. In practice, constraints mainly imposed by various sources of contamination in the laboratory and the instrument itself, as well as the need to dilute sample solutions prior to analysis ultimately limit the detection capabilities. Here we review these sources of contamination and wherever possible propose remedial strategies that we have found efficacious for ameliorating their impact on the results of multi-elemental trace analyses by ICP-MS.

(B-4)
PLASMA-BASED AMBIENT DESORPTION/IONIZATION MASS SPECTROMETRY

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The ultimate goal of analytical chemistry is to provide, what G. E. F. Lundell described as, "the chemical analysis of things as they are" such that a comprehensive assessment of sample constituents is directly obtained in a way that is nondestructive, while the sample is interrogated in its native environment. Recent efforts in mass spectrometry ionization source development have demonstrated these attributes to be possible. In such ambient desorption/ionization mass spectrometry (ADI-MS) experiments, the source desorbs molecules from a surface, softly ionizes them, and transfers these ions into a mass spectrometer. Since its inception in 2004, more than 50 different ADI sources have been described in the literature. Perhaps most surprisingly, over half of them are based on an electrical discharge. This course will cover fundamental principles of desorption/ionization processes with plasma-based sources as well as applications of these ionization sources.

(C-1)

TRACING ELEMENT METABOLISM IN ANIMALS AND HUMANS USING STABLE ISOTOPE TECHNIQUES

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Stable isotopes can be used, in principle, like radioisotopes for tracing element absorption, utilization and metabolic processes in living organisms including the human body. Over the past two decades, they have become the method of choice in metabolic studies. Health hazards associated with their use are negligible as they do not decay. However, accurate measurement of isotope ratios of trace amounts of metals is challenging. This has turned stable isotope tracing into a new research domain and application of inorganic mass spectrometry.

In this short course, participants will be familiarized in this course with the basic principles and practicalities of tracing element uptake, utilization and excretion from the body in humans and animals. This includes a basic introduction to human physiology, metabolism and bioavailability of the most relevant essential elements (iron, zinc, calcium, selenium), theoretical concepts of element tracing in living organisms based on isotope dilution principles, standard methods and protocols to study element metabolism in animals and humans, aspects to consider in the design of such studies, practicalities of sample collection and preparation as well as mass spectrometric analysis and, finally, principles and algorithms for translation of analytical data into physiological information. Participants with a background either in inorganic mass spectrometry or life sciences with an interest to conduct stable isotope studies in animals or humans are encouraged to attend. Expertise in isotope analysis and/or basic physiology is an advantage but not a prerequisite for attending the course.

(C-2)

MODELING AN INDUCTIVELY COUPLED PLASMA TORCH BY MEANS OF FLUENT: FUNDAMENTALS AND CHALLENGES

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The aim of this short course is to give an introduction how to build a computational model in order to simulate an ICP torch connected to a mass spectrometer interface. The model needs to take ionization into account (i.e., plasma formation) and should be able to trace the gas flow from the injector inlet to the sampler cone, as well as calculate the plasma characteristics inside the entire ICP torch, in the presence of a MS interface.

The whole simulation setup is divided in three major steps. The first step, i.e., pre-processing step, includes the preparation of the geometry and mesh, providing the physical equations or properties as user-defined functions and user-defined scalars, written in C, as well as defining the boundary and initial conditions. In the second step the model is solved, while the third step accounts for the post-processing or analyzing the results.

After presenting some general considerations to be used in any model, the physics of the ICP and the related equations will be discussed. More specifically, the gas flow dynamics, electro-magnetic field, source terms, ionization, and material parameters as a function of temperature and electron density will be briefly explained.

In short, the course will cover the following sections:

Modeling geometry, assumptions and input conditions

Equations to be solved in the model

Calculation strategy

Moreover, the typical errors which occur during the calculation as well as major challenges of the modeling will be discussed.
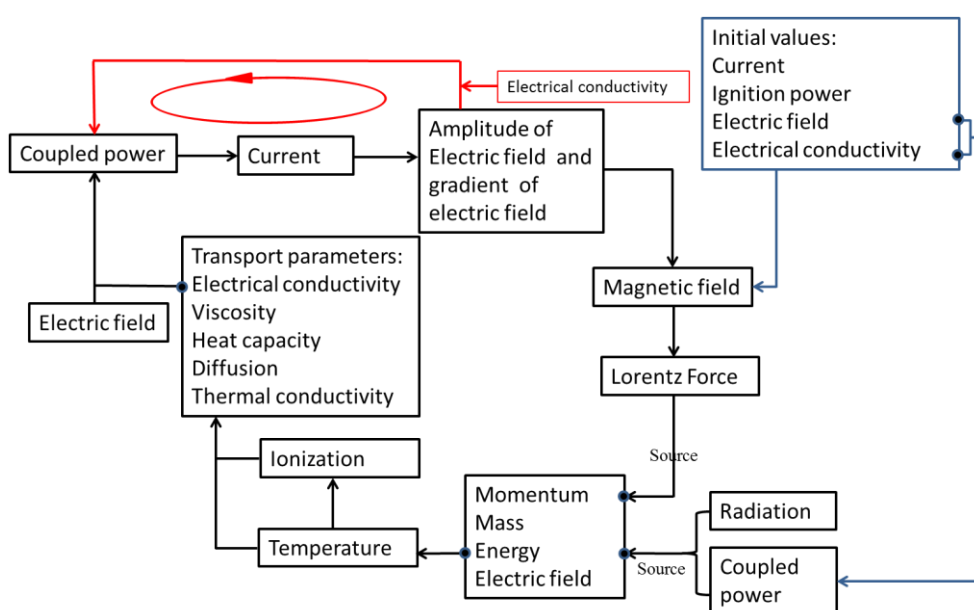
Solution strategy of the model

(C-3)

FROM SPECIATION TO METALLOMICS: RECENT ANALYTICAL APPROACHES AND QUANTIFICATION STRATEGIES USING ICP-MS

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Inductively coupled plasma-mass spectrometry (ICP-MS) represents an important tool in elemental speciation and metallomics studies. In particular, hyphenated techniques using ICP-MS as detector have proven to offer a significant insight into various metal- or metalloid-related investigations. This short course will highlight some recent examples on the use of ICP-MS in elemental speciation and metallomics including low-molecular elemental species, metalloproteins and nanoparticles in biological systems. Special attention will be paid to different quantification strategies offered by ICP-MS including internal standardisation and isotope dilution analysis being useful in elemental speciation and metallomics.

(D-1)

CHEMICAL IMAGING OF BIOLOGICAL MATERIAL: X-RAYS VERSUS PLASMA METHODS

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The different X-ray methods for chemical imaging of metals in biological materials, particularly brain tissues, will be discussed. These methods enable analysis across a range of spatial resolutions from regional to sub-cellular. Methods to be included include synchrotron X-ray fluorescence techniques for elemental imaging, X-ray absorption spectroscopy for speciation imaging, X-ray diffraction for structural imaging, phase contrast for enhanced contrast imaging and scanning transmission X-ray microscopy for spectromicroscopy analysis of organic and inorganic material. Two- and three-dimensional imaging methods will be considered. The various X-ray methods will be compared with other imaging tools, in particular with laser ablation inductively plasma mass spectrometry.

(D-2)

NANOMATERIALS CHARACTERIZATION BY ICP-MS IN SINGLE PARTICLE MODE AND RELATED TECHNIQUES

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In this short course, analytical methods based on inductively coupled plasma quadrupole mass spectrometry (ICP-MS) for ultra-trace detection of nanomaterials will be discussed. This course will cover fundamental principles of ICP-MS in single particle mode (SP-ICP-MS). Also, selected applications with and without capillary electrophoresis (CE) for particle sizing and particle fractionation will be discussed.

This course is intended for those with a background in ICP-MS but beginners are also welcome to attend.

In the first part of the course, fundamental principles of nanoparticle detection and characterization with ICP-MS in single particle mode will be discussed. The possibility of instrumental modifications to the vacuum interface will be presented as a way to improve the sampling efficiency and help detecting particles of smaller size. A particular emphasis will be placed on measurement artifacts that can arise during ICP-MS data acquisition, which – if unnoticed or uncorrected – may lead to errors in ICP-MS results and particle size histograms.

In the second part of the course it will be discussed how capillary electrophoresis can be used as a nanoparticle fractionation technique and provide complementary information on the nanoparticle size and nanoparticle coating when CE-SP-ICP-MS is used. The fundamental principle of fractionation of particles in CE will be discussed. Selected applications and limitations of the method will be critically reviewed.

(D-3)

DETECTION, IDENTIFICATION AND QUANTIFICATION OF NANOPARTICLES IN COMPLEX MATRICES: REMAINING OPPORTUNITIES FOR HYPHENATED FIELD FLOW FRACTIONATION

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Field- flow fractionation (FFF) in combination with elemental and sizing detectors has emerged as a highly promising approach for size-based elemental speciation in complex environmental samples and consumer products such as food [1,2]. Given the complexity of nano-objects and of the matrix in most real samples, the use of a single measurement technique has often resulted in their ambiguous detection and characterization. The use of a multi- method approach based on the combination of a powerful fractionation technique (*e.g*., FFF) with appropriate detection systems (*e.g*., ICP-MS, MALS, TEM, NTA, *etc*.) could prove invaluable for providing comprehensive and accurate information on the properties of target species/nano-objects. This may be useful for their unambiguous detection and characterization in complex environments.

This short course will discuss theoretical principles of FFF and practical considerations for method development and troubleshooting, in particular, for asymmetric flow FFF (AF4). The benefits of multi-method approaches using AF4 as a fractionation technique for PTA, MALS, TEM and sp-/ICP-MS detectors for the determination of size, size distribution, number based concentration and size-based elemental composition in real samples with a variety of nano-objects/species will be discussed. The potential of approaches will be demonstrated through applications to (*i*) the characterization of nanomaterials (e.g. TiO_2 and SiO_2) added to food, *(ii)* the characterization of silica nanoparticles in biological cell media relevant to nanotoxicology, *(iii)* the fractionation and characterization of plasma metalloproteins and their interaction with metallodrugs, and *(iv)* the characterisation of UV radiation filters in cosmetic sunscreen products. Special attention will be paid to the systematic development of sample preparation procedures as a trade-off between extraction efficiency and preservation of the measurand properties, also to FFF method optimization with regards to separation selectivity and nanoparticle recovery. Quality control aspects such as remaining challenges in mass balance calculations and the need of quality control or reference materials as well as of laboratory intercomparisons for method validation will also be discussed with reference to current EU projects.

[1] F. Von der Kammer, S. Legros, E.H. Larsen, K. Loeschner, T. Hofmann, *Trends Anal. Chem.* **30**, 425-436 (2011).
[2] V. Nischwitz, H. Goenaga-Infante, *J. Anal. At. Spectrom*. **27**, 1084-1092 (2012).

Keywords: complex samples, life sciences applications, engineered nanomaterials, FFF, AF4, reference nano-materials, multi-modal approaches.

14   Poster Abstracts

(P-1)

CHARACTERIZATION OF CHLORINE IN VEGETABLE OILS BY ICP-MS/MS

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Esters of 2- and 3-MCPD (monochloropropanediol) are important contaminants formed during the refining process of vegetable oils used as foods or food ingredients. Due to their quasi-complete hydrolysis to their respective free forms in the GastroIntestinal (GI) tract, 3-MCPD have been categorized as potentially carcinogenic to humans.

Many publications investigate the causality / preferential pathway of MCPD formation, depending on whether chlorine source is either organic or inorganic.

Any mitigation process tested on precursors in crude oil or MCPD in refined oils could therefore be evaluated with an analytical method allowing the total chlorine analysis in oils of interest. A method using ICP-MS/MS detection after appropriate sample preparation has been developed for total chlorine determination in crude vegetable oils, such as palm and sunflower oils. The performance of the developed method will be illustrated with data on instrumental LoD/LoQ, linearity, selectivity…

(P-2)
QUALITY ASSURANCE MEASUREMENTS WITH REFERENCE MATERIALS

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Quality assurance is an essential tool for analytical laboratory. This study contains, multi-elemental analyses of 4 different reference materials. The concentrations of given elements (B, Sr, Mo, Cd, Hg, Pd, U, Al, P, S, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, As and Se) were determined with High Resolution sector Field Inductively Coupled Plasma-Mass Spectrometer (HR ICP-MS, Element 2, ThermoScientific).

The two soil samples studied were Montana II Soil (SRM 2711a by NIST) and Gargen Soil (ISE 907 by WEPAL). The two water samples were Batch Surface Water (SS-SW2 by Spectrapure Standard) and Natural Water (SRM 1640a by NIST) respectively. Prior to analyses, the moisture content of the soil samples were determined. After that the samples were digested with strong nitric acid - hydrochloric acid - hydrofluoric acid cocktail in microwave Digestion unit (Milestone EthosUp). Some residue was observed in Montana Soil sample tubes after the digestion and additional 1 mL of strong HF was added and re-run with microwave unit was performed. Afterwards solutions were diluted by weighting to 50 mL with Milli-Q® water and furthermore with 1% HNO_3 (ULTREX II; J.T. Baker) for the analyses. The three blank samples were treated same manner as the actual soil samples. The reference water samples were diluted with 1% HNO_3 to proper concentration.

The analyses were performed with low (R ≈ 300), medium (R ≈ 4 000) and high (R ≈ 10 000) resolutions. Standard solutions, 0.1, 0.5, 1, 10, 50 and 100 ppb, were diluted from Inorganic Ventures multielement standard for ICP-MS Calibration Standards 21 and 29 with 1% HNO_3. Mercury calibration standards (0.1 ppb, 0.5 ppb, 1 ppb and 10 ppb) were diluted from SPEX ICP Laboratory performance check 1 solution. Reference Standard solution SQS-01 (AccuTraceTM) and LPC-1-100 standard solution (By SPEX) were used to prepare the control samples. All the measured solutions contained an internal standard, 10 ppb of rhodium, to control the changes in signal. The samples were injected through SeaSpray nebulizer (0.4 ml/min) and double pass spray chamber equipped with Peltier cooling unit.

The moisture content of the soil samples was determined to be 2.3 % for Garden soil and 1.9 % for Montana II soil. The elemental analyses of the water samples were in a good agreement with the reference certificate. Excluding Al, Cr, Ni and Se, the measured and actuals values differed less than 5 %. More uncertainties were discovered in the soil sample analyses. B, Hg, S, P, Se and Al were found to be particularly challenging. In general, the measured values varied 10 % from the actual values given in reference certificate. Possible sources of error could be impure acid used in the microwave digestion or the fact that the digestion was not complete. In addition, the small sample size increase uncertainties. Comparatively high B concentration measured from the samples might originate from the acid container that was borosilicate glass. In all the analyzed samples the B concentrations were 60-90 % higher compared to the actual given values. In the actual analyses, so-called memory effect might produce uncertainty and error in the results. In general, the sample digestion procedure needs further optimization.

(P-3)

INVESTIGATION OF CHEMICAL ELEMENTS REDISTRIBUTION IN PARTICLE VOLUME OF INCONEL 718 POWDER DURING THE PLASMA TREATMENT

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Austenitic high-temperature nickel-based alloy Inconel 718 is used in the production of turboshaft engine components due to its high mechanical properties at moderate and high temperatures. The alloy has a high corrosion resistance and resistance to oxidation. Manufacture of products of this alloy is performed not only by traditional methods of subtractive metal treatment, but also by advanced methods of additive manufacturing. To ensure the high quality of the products grown by the additive methods, strict requirements are imposed to the initial powder material in terms of sphericity of particle shape and uniformity of its fractional composition.

The powder produced by gas atomization methods is not sufficiently spherical and requires additional processing, which is typically carried out in an inductively-coupled plasma [1]. Plasma treatment of the powder not only changes the morphology of the surface of its particles, but also is capable of changing its physical and chemical characteristics. Plasma spheroidization of Inconel 625 increased the surface hardness of the particles in 4.5 times [2]. It was shown [3] that during the laser sintering of the powder of the Inconel 718 alloy, a spatial redistribution of the alloying elements occurs under the influence of heating in the presence of oxygen. Therefore it is of interest to investigate changes in the physical and chemical characteristics of Inconel 718 powder during its plasma treatment.

A laboratory version of a plasma-chemical reactor in argon atmosphere with a power of 40 kW and a frequency of 5 MHz was used. Electron microscopy and element analysis were carried out using the Auriga CrossBeam workstation (Carl Zeiss) equipped with an addon for the local X-ray spectral energy-dispersive microanalysis INCA X-Max (Oxford, Great Britain).

It is shown that the plasma treatment improves the sphericity of particles and makes the fractional composition narrower due to the fading of the fine fraction of the powder. Study of polished particles has revealed that a core-shell type particles with a nickel core and a shell of oxides of alloying elements are formed in presence of oxygen.

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(P-4)

INDUCTIVELY COUPLED PLASMA PROCESSING OF NICKEL ALLOYS POWDERS FOR ADDITIVE MANUFACTURING

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The powders of the nickel alloys are widely used in both traditional powder metallurgy and rapidly developing industry of additive technologies. The quality of the products obtained by the additive methods is directly determined by a set of parameters of powder particles like, for example, the sphericity and uniformity of fractional and chemical composition. During the process of the powder production by the gas atomization methods, gas pores can be formed inside the particles [1]. These faulty particles suspended in the gas can collide each other forming satellite structures of non-spherical shape. Such the particles deteriorate the quality of the powder material and reduce the durability and fatigue characteristics of the final products made of them.

That is why the development of a technology for plasma-based treatment of nickel alloy powders, improving the overall quality of the powder, is promising and practically meaningful.

A nickel-based analogue of Inconel 718 powder material was investigated in this work. Electron microscopy of the powder has shown that there are many satellites and non-spherical particles in the sample under study. Gas-filled pores within the cross-sections of particles of the initial powder are observed.

A laboratory version of a plasma-chemical reactor in argon atmosphere with a power of 40 kW and a frequency of 5 MHz was used. Electron microscopy of samples of the initial and the processed powders were carried out using the Auriga CrossBeam workstation by Carl Zeiss.

It is shown that the process of plasma treatment of raw powder makes the particle almost spherical and forces gas removal away from the particle volume. As the particle heats up, the gas pressure in the pores increases. After the material reaches its melting point, the gas-containing pores disappear due to buoyancy effects. Choose of a certain operating mode of the plasmatron can ensure a long circulation of particles in the plasma, which will allow them to degas and to spheroidize at the melting point.

(P-5)

PLASMOCHEMICAL PROCESSING OF POWDER MATERIALS FOR HEAT-PROTECTIVE COATINGS

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The increase of efficiency and durability of turboshaft engines is directly related to the effective thermal protection of working surfaces of the turbine blades and other heat-affected elements [1]. One of the ways to solve this problem is to apply heat-resistant ceramic coatings based on ZrO_2 stabilized by yttrium dioxide. This material is characterized by a low coefficient of heat conductivity λ (0.6-1.3 $W/(m^{-1}K^{-1})$) and a high (for ceramics) coefficient of linear thermal expansion α (($6\text{-}13)\cdot10^{-6}$ deg^{-1}), which is comparable with the corresponding coefficients for high-temperature nickel-cobalt-based alloys (($15\text{-}17)\cdot10^{-6}$ deg^{-1}).

Most often, ZrO_2-based coatings are deposited by means of the arc plasma spraying, although magnetron, ion-plasma and electron-beam depositions are also used. The highest coating quality is achieved using spherical-shape particles of ZrO_2.

A chopped ZrO_2 powder with particles of arbitrary geometric shape was used as the initial raw material. A laboratory ICP chemical reactor in argon atmosphere with a discharge power of 40 kW and a frequency of 5.2 MHz was used for spheroidization of the powder.

Optimization of the operating mode of the plasma-chemical reactor has been carried out to achieve the maximum efficiency of the spheroidization process. A comparative study of heat-insulating coatings obtained on the basis of the spheroidized powder and commercial powder Sulser Metco 240C was carried out. The results of the study have shown that the coating obtained using the spheroidized zirconia powder is not worse compared to the ones based on commercial powder in terms of the main parameters.

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(P-6)

NUMERICAL SIMULATION OF THE POWDER PARTICLES BEHAVIOUR IN A TECHNOLIGICAL ICP

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In early stage of ICP simulations, evolution of powders in ICP was simulated within a two-dimensional cylindrically symmetrical (2D) ICP models [1]. In our days three-dimensional non-stationary (4D) models of ICP are developed by few groups and applied for technological ICPs [2,3] (mostly for simulation of nanoparticle growth), as well as for spectrochemical ICP [4,5]. However, time of computation of the 4D models is large. For example, the 4D model developed in our group takes 2-3 days for calculation of one second of the ICP evolution (a simplified model without introduction of the sample in the plasma). This restricts application of the 4D models for practical optimization of the ICP parameters. From the other side, our 2D model reaches (for a similar simplified task) the result in about 10 minutes. Therefore the 2D models should not be forgotten yet.

Here we present a 2D model of the technological atmospheric pressure ICP. The model is based on our previous 2D ICP model, which has demonstrated a good agreement with experimental data for a spectrochemical ICP [6,7]. For this work the model is extended: axial component of the electrical current flowing in the load coil is taken into account [8]. This allows simulation of electromagnetically-driven rotation of the plasma around the axis. Evolution of the particles of the powder (trajectories, heating and evaporation) is included in the model together with thermal and gas-dynamic load of the plasma by the particles.

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(P-7)

ELECTROMAGNETIC NATURE OF VORTEXES IN TECHNOLOGICAL ATMOSPHERIC PRESSURE ICP

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An LTE-based two-dimensional (cylindrically symmetric) stationary model of ICP was developed and applied for the simulation of fundamental properties of a large size (diameter of the torch is 8.5 cm) technological atmospheric pressure ICP. The model was based originally on existing models of J. Mostaghimi, M. Boulos, P. Proulx *et al* [1] and Lindner *et al* [2], and have a good agreement with experimental data measured for a spectrochemical ICP [3,4]. Now the model is extended based on a work of Xue *et al* [5], where axial component of the electrical current in the load coil is taken into account. This allows simulation of tangential Lorentz force in the plasma and the corresponding electromagnetically-driven rotation of the plasma around the axis. The developed model is further extended to include radial component of the vector potential (which was not included in [5]). Thus the presented model includes all the main fundamental phenomena (not considering evolution of sample or powders in the plasma), which can be simulated within assumptions of cylindrical symmetry, stationarity and LTE.

It was found that the Lorentz forces in the induction zone of the ICP are significantly higher than the gas-dynamic pressure. As a result, there are two strong vortexes in the ICP, which are produced by the Lorentz forces. The 1st one rotates in *z-r* plane of the ICP. The 2nd vortex results in rotation of the plasma around the axis. The *z-r* vortex in the technological ICP prevents introduction of the powder inside the hot area of the plasma and is therefore a negative factor. Ways to reduce this vortex are discussed.

In contrast to the technological large size ICP, the Lorentz forces in the conventional spectrochemical one are negligible owing to smaller size of the ICP source. This result of our simulations is also confirmed by a similarity laws existing for ICP torches [6].

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(P-8)

COMPARISON OF TWO METHODS FOR DETERMINATION OF IODINE IN FOOD BY INDUCTIVELY COUPLED PLASMA-MASS SPECTROMETRY (ICP-MS)

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Iodine is an essential element of human nutrition. So, its absence in the diet will lead to a risk of developing iodine deficiency disorders. Therefore, it is necessary to control the content of iodine in the food products and dietary supplements.

The existing official method (EN 15111:2007) is based on the alkaline extraction by 0.5 % tetramethylammonium hydroxide (TMAH) and quantification of iodine by inductively coupled plasma-mass spectrometry (ICP-MS) technique. But the data show that a conventional microwave digestion procedure can be used to prepare samples for iodine determination by ICP-MS as routine analysis. The main aim of this work was to compare these two methods of determining iodine in food products and dietary supplements by comparing the results of extraction and detection of iodine, time of preparing of samples and solutions for analyses.

The samples were digested in nitric acid using the closed vessel microwave digestion system, the observed signal is not stable when iodine is measured by ICP/MS at m/z 127. To prevent loss of iodine the stabilizer (ammonium hydroxide solution) was added immediately after digestion, then filtered and analyzed. Te (m/z 130) was used as an internal standard.

In 2017 the nitric acid digestion method was tested in two proficiency tests (FAPAS 1889 - infant formula, FAPAS 1891-milk powder), z-score were «-0.1» and «-0.4» respectively.

Both these methods showed good precision and trueness, the levels of recovery of the iodine were $(98 \pm 10\%)$ for HNO_3 and (95 ± 10) % for TMAH.

Accuracy and recovery were evaluated using standard reference materials ERM BB 422 (fish muscle) and Fapas 1891 (milk powder).

The high recovery and accuracy are sufficient for the quantitative analysis of the iodine by both methods.

(P-9)
NEW FRONTIERS IN BIO-MONITORING – TOTAL AND SINGLE PARTICLE ANALYSIS

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For many years the ICP-Mass Spectrometry is a tool of choice for the trace analysis of elements like Pb, As, Hg, and Cu in body fluids such as urine, blood, serum and saliva as well as in tissues. Single elements or panels of toxic or nutritional elements are run in the these matrices providing doctors with comprehensive views on patient conditions.

The goal of this presentation is to demonstrate the research capability of the current ICP-MS technology for trace element analysis in body fluids. A winning combination of reaction/collision spectral interference removal allows for the accurate determination of the low levels of analytes of interest.

Recently, due to the popularity of implants, elements like Ti and Co were added to the common list of tested analytes. They are nontoxic, but can give medical providers information on an implant degradation. It will be shown that the current ICP-MS technology can assess implants degradation level not only by measuring the total Ti content but also by using the single particle technique. The single particle ICP-MS offers a better understanding of the degradation process of implants and an improved detection limits allowing earlier diagnosis.

In summary, the ICP-MS, in combination with an optimized sample introduction system, is a perfect technique for the analysis of diverse types of biological matrices including urine, serum and blood for total concentration and single particle analysis. One simple sample preparation technique, the appropriate diluent, and panels or individual analytes can be measured quickly and precisely. The results in reference materials will be shown and discussed.

(P-10)

LASER ABLATION-HALO-FLOWING ATMOSPHERIC PRESSURE AFTERGLOW-MASS SPECTROMETRY FOR SPATIALLY RESOLVED ANALYSIS OF ACTIVE INGREDIENTS IN PHARMACEUTICAL TABLETS

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Mass spectrometry imaging (MSI) has become a valuable tool for the measurement of spatial distributions of target analytes in complex samples. Most often, MSI of molecular species is performed with matrix-assisted laser desorption/ionization (MALDI) and secondary ion mass spectrometry (SIMS). Due to the requirements of these methods, molecular MSI is reliant upon cumbersome sample preparation, partly due to the fact that the sample is analyzed in the vacuum of the mass spectrometer. The focus of this work lies on the development of a new molecular imaging technique that combines the good spatial resolution and reproducibility of sample introduction provided by a laser ablation system with a novel ambient ion source, the halo-flowing atmospheric pressure afterglow (halo-FAPA) and its application for spatially resolved analysis of pharmaceutical tablets.

For this purpose, sample material was ablated from two different pain killer tablets with a 213 nm wavelength Nd:YAG laser and transported to the ion source in a nitrogen carrier gas stream. An in-house assembled halo-FAPA with an optimized geometry was used for the ambient desorption/ionization of analyte molecules from sample particles by passing the generated aerosol from the laser ablation chamber through the inner capillary of the FAPA source. For optimization, different experimental parameters such as the discharge and carrier gas flow rates and the discharge current were tuned. The setup was subsequently employed to investigate the heterogeneous distributions of active ingredients in pharmaceutical tablets with a spatial resolution of around 25 µm. The FAPA ion source could be easily coupled with different types of mass spectrometers, which allowed the identification of active ingredients *via* their exact mass as well as their distinctive fragmentation pattern. The results of these imaging experiments indicate that the spatial distribution of active ingredients in pharmaceutical tablets can give information as to their authenticity and origin and thus could be useful for the identification of counterfeit pharmaceuticals.

(P-11)

ELEMENTAL CHARACTERIZATION ANALYSIS OF DECOMMISSIONING MATERIALS FROM FIR1 TRIGA MARK II TYPE RESEARCH REACTOR

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VTT Oy has, TRIGA Mark II type (General Atomics) research rector, FIR1 that has been used for training, isotope production, BNCT treatments and activation analysis from 1962 to 2015. In June 2015, the reactor was shut down and planning of its decommissioning was started. According to Finnish nuclear and radiation safety regulatory guides, scaling matrix approach is used for FIR1 decommissioning. Each material and waste type are characterized prior to dismantling and so-called nuclide vectors and gamma active key nuclides are defined. During the dismantling, only key nuclides in waste packages are determined by gamma spectrometry. The inventory of hard-to-measure beta nuclides can be scaled for each waste package when the similar nuclide ratios in certain waste matrix are assumed. Prior to decommissioning of FIR1, all different reactor materials and waste types are characterized in order to define radionuclide inventories in different materials and waste streams. Characterization enables planning of safe dismantling and packaging of decommissioning wastes. It also helps planning of interim storage and later final disposal in a way that they are safe, their radiological impact can be predicted and they are according to legal requirements. Characterization of FIR1 reactor includes modelling the radiochemical inventories, and verification and validation of inventory calculations via analyses of material's original chemical composition and radiochemical analyses. [1]

As a part of FIR1's waste and material characterization, original chemical composition of different reactor materials has been analysed with High Resolution sector Field Inductively Coupled Plasma-Mass Spectrometer (HR ICP-MS, Element 2, ThermoScientific). Prior to HR ICP-MS analysis, suitable pre-treatment and dissolution method for each material was tested and selected. Elemental analyses were performed from diluted sample solutions. Calibration curve and control samples were diluted from ICP-MS Multi-Element Solutions by SPEX, Inorganic Ventures and AccuTrace^{TM} standard solutions. All measured solutions contained an internal standard; 10 µg/L of indium or rhodium, to control the changes in signal. The samples were injected through SeaSpray nebulizer (0.4 ml/min) and double pass spray chamber equipped with Peltier cooling unit. Aluminium sample cone and Nickel skimmer cone were used during the measurement. Elemental composition of lead, aluminium and graphite samples has been analysed with HR ICP-MS equipment, so far. In order to determine the nuclide vectors, the characterization analyses of materials from various parts of reactor with different radionuclide inventory will be analysed in the future.

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(P-12)
TOTAL ELEMENTAL ANALYSIS OF FOOD SAMPLES WITH ICP-OES AND ICP-MS

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The measurement of toxic, essential and nutritional elements in food has, through regulatory drivers and todays health-conscious consumers, become a routine part of food quality monitoring. Alongside regulatory compliance, it is necessary to monitor potentially toxic contaminants that could enter the food chain via a series of pathways including, but not limited to, industrial pollution or environmental contamination. For these reasons, it is essential to have a simple, robust, multi-elemental analysis method for detecting and quantifying major and minor concentrations of elements in food.

ICP-OES and ICP-MS are sensitive and rapid techniques with wide linear dynamic range and as such are ideal tools for the analysis of trace and major analytes in food together in one analytical run. The principal challenge for trace elemental ICP-based techniques are interferences that stem from the complex food matrix, the reagents used to prepare the sample and the plasma source. This paper reviews different strategies, including collision/reaction cell (CRC) approaches in triple quadrupole ICP-MS, for the accurate analysis of trace elements in food sample matrices. The accuracy of the techniques reviewed is demonstrated by the analysis of food based certified materials following microwave digestion.

(P-13)

INVESTIGATING ELECTRICAL CONTACT LOSS WITHIN LITHIUM ION BATTERY ELECTRODES BY MEANS OF SINGLE PARTICLE ANALYSIS WITH ICP-OES AND -MS

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Lithium ion batteries (LIBs) are the most commonly used electrochemical energy storage technology not only for small portable devices but also for electrical vehicles. There are many research activities aiming on the one hand to develop new battery materials and on the other hand to deepen the understanding of already established materials. One of the major research fields is the elucidation of causes for capacity fading. Electrical contact loss of active material particles is frequently stated as one of the reasons for a capacity decrease but there are no experimental studies found on this topic. Most studies consider battery electrodes as a whole and provide mean values as results. However, investigations on this issue require a resolution on a particle level.
During electrochemical cycling of LIBs the anode and cathode active materials are lithiated and delithiated by turns. Under open circuit conditions, all electrically connected particles have the same degree of lithiation which is mostly determined by the electrode potential. In contrast, the particles that lost their electrical contact should exhibit degrees of lithiation according to the electrode potential of the moment at which the contact loss occurred. Therefore, the distribution of the lithiation degree provides information on the extent of electrical contact losses inside of a LIB electrode.

From a thermodynamic point of view, an electrode with particles of different lithiation degrees can be considered as a non-equilibrium system. This state needs to be maintained during sample handling. Avoiding liquids, for example, by a direct aerosol sample introduction appears to be beneficial to minimize the risk of a regain of electronic and ionic conduction between the particles. ICP-OES and -MS techniques are the methods of choice to determine elemental ratios of single particles of the sampled aerosols. The aerosol sample introduction enables a particle size separation by using an adjustable upward gas stream. This helps to identify events of simultaneous introduction of more than one particle.

Since common LIB active material particles are rather large (approximately 1-10 µm) the challenge of this application is not a sensitivity issue but to guarantee a complete or at least representative ionization and excitation.

(P-14)

ANALYSIS OF ORGANOPHOSPHORUS AGING PRODUCTS IN LITHIUM ION BATTERY ELECTROLYTES *VIA* GC-ICP-SF-MS AND GC-EI-MS

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Since established in many both mobile and stationary applications, lithium ion batteries (LIBs) have to meet challenging demands. On the one hand, high power, high capacity and long lifetime have to be accomplished, on the other hand, safety cannot be neglected. Therefore, comprehensive knowledge of reaction mechanisms of battery components during cycling is important. Today's state-of-the-art battery systems use lithium hexafluorophosphate (LiPF$_6$) as conducting salt dissolved in a mixtures of cyclic and linear organic carbonates. Since the salt is highly hygroscopic, trace-amounts of water are always present in the battery system. The ionic form of the dissolved salt is in constant equilibrium with LiF and PF$_5$. The latter can undergo decomposition reactions with water and the organic carbonates eventually forming organophosphorus compounds and hydrofluoric acid.

These organo(fluoro)phosphates show structural similarity to chemical warfare agents like sarin and therefore have a supposedly high toxicity due to a similar metabolism in the human body. Even though only present in relatively low concentrations in laboratory scale cells, the quantity in mobile and stationary applications becomes significant when larger amounts of electrolyte are implemented. In previous investigations, a large variety of organophosphates could be qualified in different electrolyte systems [1]. A major drawback is the lack of commercially available standards for those compounds which makes quantification using molecular investigations difficult. In this study, an inductively coupled plasma-sector field-mass spectrometer (ICP-SF-MS) is used to quantify organophosphorus compounds of the LIB system. Speciation of compounds was performed *via* gas chromatography (GC) techniques. Identification of the electrochemically formed LiPF$_6$ decomposition products was performed using gas chromatographic separation and electron ionization-mass spectrometry (GC-EI-MS) in order to obtain molecular information using spectral database comparison of characteristic fragmentation.

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(P-15)

SPECIATION OF POTENTIAL TOXIC DECOMPOSITION PRODUCTS IN LITHIUM ION BATTERY ELECTROLYTES BY COMBINATION OF HPLC-ION TRAP TIME OF FLIGHT-MS AND HPLC-ICP-MS

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The improvement of lithium ion batteries (LIBs) is one major demand for the continuous progression of electro mobility. Therefore, higher energy density, enhanced cycling stability, increased cell voltage as well as a high C-rate stability are desirable to become competitive against combustion engines. These challenges for automotive application push the electrolyte to the limit concerning fast charge and discharge (thermal stability) and high-voltage cathode materials (oxidative decomposition).

Today's state-of-the-art LIB electrolyte consists of the conducting salt lithium hexafluorophosphate ($LiPF_6$) dissolved in a mixture of linear and cyclic organic carbonates. From the first charge the electrolyte starts to decompose due to the thermal and chemical instability of the P-F bond. Consequently, the reactive intermediate PF_5 undergoes reactions with organic solvent and trace amounts of water in the cell leading to highly diverse fluorinated and alkylated phosphorus-based decomposition products after a reaction cascade.[1]
These products show structural similarity to pesticides and chemical warfare agents which implies the need of toxicological investigation, especially regarding cell setups with high electrolyte amount in the range of several liters like hybrid electric vehicles (HEV) or stationary storage units. Over 20 acidic as well as non-acidic species of organophosphates (OPs) and organic fluorophosphates (OFPs) could be identified in LIB electrolyte aging experiments with separation techniques like gas and ion chromatography.[2,3]

In contrast, high performance liquid chromatography (HPLC) allows the separation of the whole OP/OFP spectra with one system by using two orthogonal separation techniques, namely hydrophilic interaction liquid chromatography (HILIC) for ionic species and reversed-phase chromatography (RP) for non-ionic products. The high structural analogy of these reaction products requires baseline separation for explicit identification as well as for the quantification with an ICP-MS.

In this work, LIB electrolyte from field-tested HEV were investigated with HPLC-ion trap time of flight-MS and HPLC-ICP-MS to gather qualitative and quantitative information about acidic as well as non-acidic phosphorus aging products. This data is taken into account to create a safety estimation for LIB electrolyte in automotive application regarding the generation of toxic byproducts during operation.

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(P-16)

VISUALIZING ELEMENTAL DEPOSITION PATTERNS ON GRAPHITE ANODES FROM LITHIUM ION BATTERIES: A LASER ABLATION-INDUCTIVELY COUPLED PLASMA-MASS SPECTROMETRY STUDY ON FACTORS INFLUENCING THE DEPOSITION OF LITHIUM, NICKEL, MANGANESE AND COBALT

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The lithium ion battery (LIB) technology, introduced in the early 90's, opened a whole new market for high power and high energy portable devices. Recent applications in the electromotive industry as well as in the field of stationary storage systems for a more efficient use of renewable energies attracted the LIB technology.

The state of the art lithium ion battery consist out of graphite anodes and mostly layered lithium metal oxide ($LiMO_2$) cathodes. One of the most interesting layered lithium metal oxides is $LiNi_{1/3}Co_{1/3}Mn_{1/3}O_2$ (NCM 111) as cathode material which show several desired properties such as high capacity, less toxicity, lower cost and milder thermal instability in the charged state. Nevertheless, depending on the application LIBs still show severe drawbacks, especially the limited storage lifetime (= calendar life) and cycling lifetime (= cycle life). These criteria are closely related to the degradation of the battery cell components, which is known as cell aging. The dissolution of transition metals from the cathode is proposed to have a major influence on the cycle life due to the deposition of those metals on the graphitic anode. It has been shown for lithium manganese oxide ($LiMn_2O_4$) spinel type cathodes that the deposition of manganese leads to cracking and contamination of the solid electrolyte interphase (SEI) and thus to ongoing lithium consumption

In this study, laser ablation-inductively coupled plasma-mass spectrometry (LA-ICP-MS) was applied to previously aged carbonaceous anodes from lithium ion batteries (LIBs). These electrodes were treated by cyclic aging in a lithium ion cell set-up against NMC111 to elucidate factors that influence transition metal dissolution (TMD) of the cathode and subsequent deposition on the anode. The investigations were carried out by qualitatively visualizing the ^7Li and TM patterns (^{60}Ni, ^{55}Mn and ^{59}Co) of whole coin and pouch-bag electrodes.

(P-17)

DETERMINING THE MIGRATION OF LITHIUM IN AGED LITHIUM ION BATTERIES BY PERFORMING AN ISOTOPE DILUTION ANALYSIS COMBINED WITH DIFFERENT PLASMA-BASED TECHNIQUES

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The growing demands for renewable energies and the urge of reducing the human ecological footprint increases the attention for lithium ion batteries (LIBs) for mobile and stationary use. While being a technology originating from in 1991 by Sony[1], the state-of-the-art LIB uses carbonaceous materials and lithium transition metal oxides ($LiMO_2$; $M = Ni_x$, Co_y, Mn_z (x+y+z=1)) as the negative and positive electrodes, respectively.

One major drawback of this technique is the subsequent capacity loss during operation. The formation in the first cycle and the ongoing growth of the solid electrolyte interphase (SEI) on the anode and the cathode electrolyte interphase (CEI) on the cathode are some of the reasons for these losses. These interphases form on the electrodes due to surface reactions because of reductive/oxidative potentials by decomposition of the electrolyte and therefore consumption of active lithium that cannot be utilized for electrochemical processes.[2]

Therefore, plasma-based mass spectrometric techniques are used in this work to analyze different components of LIBs, aged under charge/discharge conditions. In detail, a ^{6}Li-enriched electrolyte was prepared to perform an isotope dilution analysis (IDA). Additionally, the electrodes are measured by inductively coupled plasma-mass spectrometry (ICP-MS) for bulk analysis and glow discharge-sector field-mass spectrometry (GD-SF-MS) for depth-resolved IDA. The electrolyte is analyzed by ICP-MS, as well. These techniques will provide a better understanding of the processes behind the SEI/CEI formation and whether the decomposed lithium originates only from the electrolyte or from the positive electrode, as well.

The cycling experiments are conducted at different charging rates and numbers of cycles for MCMB/NCM622 ($LiNi_{0.6}Co_{0.2}Mn_{0.2}O_2$) full cells.

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(P-18)

MATRIX-MATCHED STANDARDS FOR GLOW DISCHARGE-SECTOR FIELD-MASS SPECTROMETRY FOR THE ANALYSIS OF LITHIUM ION BATTERY ELECTRODES

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One postulated cause of the degradation of lithium ion batteries (LIBs) is assigned to the passivation layer on the negative electrode which is formed during the first cycle due to high reductive potentials. This passivation layer is called solid electrolyte interphase (SEI) and grows with ongoing cycling and consumes active lithium which results in capacity losses. Furthermore, the dissolution of transition metals - originating from the positive electrode – was proposed to have an negative influence on the SEI as it affects the surface of the passivation layer.[1] The conventional method to examine passivation layers in battery research is the use of X-ray Photoelectron Spectroscopy (XPS) which suffers from poor depth resolution as well as long measurement times due to small sample spots as well as the low sample throughput.[2]

Due to a lack of reliable methods for micrometer scale determination of the elemental distribution in aged lithium ion electrodes as well as a lack of suitable certified reference standards, standard electrodes for the calibration of plasma based depth-and spatially-resolved methods were developed. Afterwards, the solid electrode standards were adapted to Glow Discharge-Sector Field-Mass Spectrometry (GD-SF-MS).

Considering the cathode/anode active material combination of $LiNi_{1/3}Co_{1}/3Mn_{1/3}O_2$ (NCM) and graphite as a standardized and well-known setup for LIB[3], the synthesized NCM/graphite composite allows to quantitatively study the lithium content in a low micrometer range on the surface and inside the bulk material of the anode. In order to examine the effect of SEI growth and transition metal deposition on negative electrodes, the GD-SF-MS is a promising tool for the direct analysis of these layers.

In this work, self-prepared matrix-matched standards are used to calibrate the GD-SF-MS externally on typical elements present in LIBs (lithium, manganese, cobalt and nickel). The validation was performed via bulk analysis of the element spiked electrodes using ICP-OES as well as characterization using LA-ICP-MS.

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[2] P. Niehoff, S. Passerini, M. Winter, Langmuir, 2013, 29, 5806–5816.
[3] M. Evertz, F. Horsthemke, J. Kasnatscheew, M. Börner, M. Winter, S. Nowak, J. Power Sources, 2016, 329, 364-371.

(P-19)

A LASER ABLATION ICP-OES METHOD FOR THE INVESTIGATION OF LITHIUM AND TRANSITION METAL DEPOSITIONS FROM LITHIUM ION BATTERY ELECTRODES

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The loss of performance of state-of-the-art Lithium Ion Battery (LIB) is still an unsolved issue. Nowadays, the demand for more powerful and long-lasting LIBs in portable electronics or for electro mobility is increasing. Understanding deterioration processes and mechanisms (the so called aging) requires the examination of aged cells. Changes in the distribution of lithium or transition metal deposition in the LIB can have a huge impact on the cycle and calendar life of cells. As electrochemical cells and especially electrodes do not age homogeneously and electrochemistry in general is heavily dependent on surface properties, bulk analysis is not suitable for investigating these phenomena. However, the understanding of these aging phenomena in LIBs is a crucial factor for current and future LIBs.

The state-of-the-art LIB consist of graphite anodes and mostly layered lithium transition metal oxide ($LiMO_2$) cathodes. One of the most interesting layered lithium metal oxides is $LiNi_{1/3}Co_{1/3}Mn_{1/3}O_2$ (NCM 111) as cathode material which shows several desired properties such as high capacity, little toxicity, low cost and little thermal instability in the charged state. It has been shown that the deposition of manganese leads to cracking and contamination of the solid electrolyte interphase (SEI) and thus to ongoing lithium consumption.
Therefore, a method using ablation-inductively coupled plasma-optical emission spectrometry (LA-ICP-OES) was developed. Solid samples were investigated using a 193 nm ArF Excimer and a 213 nm Nd:YAG Laser, respectively.

Due to a lack of commercially available solid standard materials we developed matrix-matched solid standard materials with a known content of analytes. The investigations were carried out by visualizing the Li and transition metal depositions (Ni, Mn and Co) of whole coin and pouch-bag cells.

(P-20)

DECIPHERING THE LITHIUM ION MOVEMENT IN LITHIUM ION BATTERIES: DETERMINATION OF THE ISOTOPIC ABUNDANCES OF ^{6}LI AND ^{7}LI VIA HIGH RESOLUTION ICP-OES FOR AGING ANALYSES

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The lithium ion battery (LIB) was first commercialized by Sony in 1991.[1] The state-of-the-art technology consists of carbonaceous materials and lithium transition-metal oxides (LiMO_2; M = Ni$_x$, Co$_y$, Mn$_z$ ($x+y+z=1$)) as the negative and positive electrodes, respectively. While the performance and capabilities of LIBs are growing rapidly, the technology has drawbacks concerning an inferior and decreased lifetime because of aging induced decomposition mechanisms. Exemplary, one of those is accounted to the loss of active lithium during the first charge/discharge cycle by forming a passivation layer on the negative electrode, the solid electrolyte interphase (SEI). During cycling, this layer consumes lithium irreversibly, which cannot be used for charge/discharge processes. [2]

Hence, an isotope dilution analysis (IDA) was performed with a ^{6}Li-enriched electrolyte to determine the migration and accumulation of lithium isotopes that are lost during the aging. However, these analyses depend typically on expensive analytical devices. Therefore, a method to determine the isotopic ratios of lithium by using high resolution inductively coupled plasma-optical emission spectroscopy (ICP-OES) is presented in this work. It was proven that the emission lines of light elements are shifted, [3] if the isotopic ratios are artificially changed. For this reason, external calibrations with different lithium isotope ratios are prepared to determine the concentration and the isotopic ratios of aged battery components.

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(P-21)

QUANTIFICATION OF DISSOLVED MN2+/3+ IN LITHIUM ION BATTERY ELECTROLYTES BY MEANS OF CE/ICP-MS – A NEW APPROACH FOR THE INVESTIGATION OF TRANSITION METAL DISSOLUTION FROM CATHODE MATERIALS

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Lithium transition metal oxides containing manganese amongst others are commonly used as cathode materials in Lithium Ion Batteries (LIBs). It is claimed that excessive manganese dissolution from the cathode has a strong negative effect on battery lifetime.[1]
Evertz *et al*. showed that transition metal dissolution from layered lithium nickel manganese cobalt oxide can be a result of material defects and also of lattice stress resulting from lithium insertion and de-insertion.[2] Additionally, Mn^{3+} in the structure can disproportionate to soluble Mn^{2+} and Mn^{4+}.[3] The disproportionation reaction mainly occurs for the spinel lithium manganese oxide (LMO) due to the redox active Mn^{3+}.

In 2015, Jarry *et al*. found soluble Mn^{3+} complexes on the surface of the spinel lithium nickel manganese oxide (LNMO).[4] In a study from 2016, the presence of Mn^{3+} in the electrolyte was confirmed in the case of LMO and LNMO.[5]

These studies show that the dissolution behavior of transition metals, especially manganese, is not fully understood and needs further investigation concerning the dissolved transition metal species. Quantification of soluble Mn^{3+} is challenging due to the favored disproportionation reaction to Mn^{2+} and Mn^{4+} and because of its high redox potential.
In this work, a CE-ICP-MS method for simultaneously identification and quantification of soluble Mn^{2+} and Mn^{3+} amongst other transition metals was developed. To achieve the separation of both manganese species, diphosphate was used as an auxiliary ligand in CE running buffer. It has the highest ability to stabilize Mn^{3+} regarding the preferred disproportionation reaction and is stable against the high redox potential of Mn^{3+}.

Different dissolution experiments with LNMO-based cathodes were performed and the recovered electrolytes were investigated afterwards regarding the dissolved manganese species.

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[2] M. Evertz et al., *J. Power Sources* **2016**, *329*, 364-371.
[3] M. M. Thackeray *et al*., *Mater. Res. Bull.* **1984**, *19*, 179-187.
[4] A. Jarry *et al*., *J. Am. Chem. Soc*. **2015**, *137*, 3533-3539.
[5] Y. Shilina *et al.*, *Anal. Chem.* **2016**, *88*, 4440-4447.

(P-22)

DETERMINATION OF ESSENTIAL AND NON-ESSENTIAL ELEMENTS IN BLOOD SERUM BY Q-ICP-MS

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The quantification of essential and non-essential elements is an important issue of the human or animal's health status assessment. In this study, we developed the method for determination of 19 trace elements and minerals (Al, As, Ba, Be, Cd, Co, Cr, Cu, Fe, Mg, Mn, Ni, Pb, Se, Tl, Th, U, V, and Zn) in blood serum using quadrupole inductively coupled plasma mass spectrometry (Q-ICP-MS) after microwave digestion with nitric acid (HNO3) and hydrogen peroxide (H2O2) solution.

The described method was validated according to the requirements of PN-EN ISO/IEC 17025:2005 and the Eurachem Guide. The following validation parameters were calculated: linearity, limits of detection (LOD) and quantification (LOQ), precision and accuracy. The LOD and LOQ were calculated based on standard deviation of spiked blank matrix. The LOQ ranged from 0.1 (As, Co, Cd, Cr, Pb, U, V) to 270 (Mg) µg/l. The precision was assessed using the coefficient of variation and accuracy was evaluated by recoveries in available certified reference materials (CRMs). Obtained results of recovery study in Seronorm L-2 ranged from 87,5 % (Se) to 124% (Ba). Estimation of uncertainty was performed using data of precision study and accuracy evaluation according to the NORDTEST 537 Guide using the MUkit software.
Reliability of results obtained within described method was verified by the analysis of spiked samples and CRMs. The obtained results of validation study confirmed that described method is suitable for the measurement of trace elements and minerals in blood serum.

(P-23)

OFFSHORE WIND CONSTRUCTIONS: CORROSION PROTECTION AS A NEW POTENTIAL SOURCE OF INORGANIC CONTAMINANTS INTO THE MARINE ENVIRONMENT?

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The offshore wind farms in the German North Sea and Baltic Sea are part of the renewable energy transition in Germany. The German government has set the aim to expand the offshore wind energy production from currently (2017) 4749 MW to 15000 MW until the year 2030. The impact of offshore constructions on the marine environment, however, remains unclear in many aspects. Especially little is known about potential emissions from corrosion protection systems used for offshore structures.

A widely used and established method of corrosion protection, besides organic coatings, are galvanic anodes composed of Al and Zn alloys. By definition, the constituents of these anodes are "sacrificed" instead of the structural steel. Hence, the application of galvanic anodes (approx. 250 kg Al-anode material per pile and year) results in the continuous emission of inorganic matter into the marine environment.

In order to evaluate the emission load from corrosion protection used by offshore wind farms, suitable tracers need to be identified and reliable analytical methods have to be developed and applied in particular to allow a differentiation against other anthropogenic sources and natural background levels.

In our study, we characterized anode material from several manufactures by ICP-MS/MS in order to identify potential inorganic tracers for emissions from offshore wind farms. The determination of these tracers in the marine environment, especially in the seawater matrix, is challenging as the released components such as In, Pb and Cd occur in concentrations of a few ng L^{-1} and less. This poster contribution will present an new extended method for the analysis of trace elements in the seawater matrix based on the coupling of the ESI sea*FAST* system to an Agilent ICP-MS/MS. First results from the method optimization as well as their application on the analysis of real samples originating from different wind farms installed in selected regions of the German North Sea will be presented.

(P-24)

LEAD ISOTOPE RATIOS FOR POLLUTION SOURCE APPORTIONEMENT IN DIFFERENT COMPARTMENTS OF THE MARINE ENVIRONMENT

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Lead is a non-essential toxic element that at high levels of human exposure causes damage to almost all organs of human body. This element naturally occurs in the Earth crust but its biogeochemical cycle has been altered by anthropogenic activities which have introduced high amount of this element from different sources. Among inorganic contaminants, Pb is perhaps the most studied, but the determination of its total concentration only is not sufficient for a proper evaluation of contamination sources. Discrimination of anthropogenic and geogenic lead sources requires both precise and accurate isotope ratio determination as well as high versatility due to the complexity of environmental matrices, such as sediments, biota and seawater. This element has a partially radiogenic isotopic composition with ^{208}Pb, ^{206}Pb and ^{207}Pb originating from the radioactive decay of ^{238}U, ^{235}U and ^{232}Th respectively and ^{204}Pb representing the only natural stable isotope. This characteristic isotopic composition represents a powerful analytical tool as it allows to trace the sources, fate and effects of possible Pb contamination. In earth science the most common way to express the Pb isotopic composition is using the ratio $^{206}Pb/^{207}Pb$ because of the easy interference-free determination and isotopes' abundance. Nevertheless, normalization to ^{204}Pb, the only natural Pb isotope, is often preferable as it allows the largest variability between reservoirs. Unfortunately, the determination of ^{204}Pb by ICP-MS is quite challenging as this is also the least abundant among Pb isotopes (about 1.4%) and it is also affected by isobaric interference from ^{204}Hg. The latter derives from both sample matrices and from plasma/ sweep gas supplies and it represents a big analytical problem especially for marine biota samples, where the amount of Hg can be up to 100 times higher than Pb.

In this work we present the development and the application of analytical protocols for the accurate and precise determination of Pb isotope ratios by HR-ICP-MS in different marine environmental matrices (sediments, seawater and biota). In the case of biota samples, a procedure involving matrix separation was included, to separate Pb from sample matrix and from Hg, present in the sample. For seawater samples, the use of the SeaFAST automated system allowed simultaneous matrix separation and analyte pre-concentration before ICP-MS analysis. A comparison with results obtained by MC-ICP-MS in the same samples was also performed and in all cases a good agreement was found with results obtained by HR-ICP-MS. Sediment samples from Caribbean, Baltic and Namibian coasts, biota samples from Mediterranean coast and Polynesia, seawater samples from Mediterranean and Arctic seas were involved in this study. The results showed how powerful this analytical tool can be in the field of marine environmental science.

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LEAD ISOTOPE RATIOS FOR POLLUTION SOURCE APPORTIONEMENT IN DIFFERENT COMPARTMENTS OF THE MARINE ENVIRONMENT

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Lead is a non-essential toxic element that at high levels of human exposure causes damage to almost all organs of human body. This element naturally occurs in the Earth crust but its biogeochemical cycle has been altered by anthropogenic activities which have introduced high amount of this element from different sources. Among inorganic contaminants, Pb is perhaps the most studied, but the determination of its total concentration only is not sufficient for a proper evaluation of contamination sources. Discrimination of anthropogenic and geogenic lead sources requires both precise and accurate isotope ratio determination as well as high versatility due to the complexity of environmental matrices, such as sediments, biota and seawater. This element has a partially radiogenic isotopic composition with ^{208}Pb, ^{206}Pb and ^{207}Pb originating from the radioactive decay of ^{238}U, ^{235}U and ^{232}Th respectively and ^{204}Pb representing the only natural stable isotope. This characteristic isotopic composition represents a powerful analytical tool as it allows to trace the sources, fate and effects of possible Pb contamination. In earth science the most common way to express the Pb isotopic composition is using the ratio $^{206}Pb/^{207}Pb$ because of the easy interference-free determination and isotopes' abundance. Nevertheless, normalization to ^{204}Pb, the only natural Pb isotope, is often preferable as it allows the largest variability between reservoirs. Unfortunately, the determination of ^{204}Pb by ICP-MS is quite challenging as this is also the least abundant among Pb isotopes (about 1.4%) and it is also affected by isobaric interference from ^{204}Hg. The latter derives from both sample matrices and from plasma/ sweep gas supplies and it represents a big analytical problem especially for marine biota samples, where the amount of Hg can be up to 100 times higher than Pb.

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(P-26)
ANALYSIS OF ELEMENTS DISTRIBUTION IN THE OMBROTROPHIC PEAT PROFILE BY ICP-MS

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It is well known, that ombrotrophic marshes are one of the key markers of atmosphere pollution by Trace and Toxic elements. Due to the specific formation of upper layers of peat they are separated from any sources of trace elements, except atmosphere, by the water level (30 – 60 cm). In upper layer pollutants are accumulated by plants and stored in their organisms prior to it decomposition. *Sphagnum* species are the most common peat-forming plants. Its decomposition releases a great number of organic substances which can retain elements by forming the covalent and coordinate bonds. Retained elements along with the decomposed biomass are transferred to deeper layers during the vegetation period as long as they rich the water level. At the water level elements, which is bonded with water soluble Fulvic acids can be removed from marshes to the ecosystem, whereas elements bonded by non-soluble in water Bitumen and Humin part and alkaline-soluble Humic substances are retained in peat profile.

Thus, the study of elements distribution throughout the peat layers will provide an information about the historical impact of human activities in trace and toxic elements atmosphere pollution. While analysis of trace elements accumulation by peat components (fulvic and humic acids, humin and bitumen) will give a vision of pollutants mobility.

The target of research was an ombrotrophic marshes peat collected throughout the depth of a genetically homogeneous deposit (0, 0 – 5, 5 – 25, 25 – 75, 75 – 125 and 165 – 215 cm). The samples were collected in the territory of the Ilass marshes in the Primorskiy district of the Arkhangelsk region, 64° 20′ 2.75″ N, 40° 36′ 33.75″ E. This territory is a common type of Pribelomorskiy province peatland, which covers a significant part of the Arkhangelsk region and neighboring territories.

Extraction of peat components was carried out by sequential extraction, which included 3 stages: bitumen extraction by butyl acetate in Soxhlet apparatus, Humic substances alkali extraction by 0.1 M NaOH in nitrogen atmosphere and separation of Fulvic and Humic acids by acidifying the humic substances solution. Peat and peat components were treated by microwave digestion procedure and estimated on ICP-MS Bruker Aurora Elite (USA).
The maximum content of trace elements is found in the upper layers of the peat profile (0 – 75 cm) and decreases significantly in layers under the water level. The distribution of elements throughout the peat components showed that only As forms complexes with bitumen part and account for 25% of its total concentration. More than a half of Zn and Fe total concentration is bounded with humin part. Co and Cu relate to the elements typically bonded with humic and Al and Se with fulvic acids.

(P-27)

ESTIMATION OF SPATIAL DISTRIBUTION OF PB AND CD IN NORTHERN TAIGA SOIL BY THE METHOD OF ICP-OES

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Procedure of assessing the contamination degree of soil cover should take into account features of the landscape in which soils are formed. In conditions of humid soil formation, distribution of heavy metals that are mobile in an acidic environment has a significant influence of the landscape exerts subordination degree. In these conditions exist the possibility of local anomalies formation with increased and decreased concentration of pollutants.

In order of evaluation of Pb and Cd spatial distribution in upper horizon of podzolic soil in northern taiga (Arkhangelsk region, Russia), samples were taken on the shore of Radnitsa lake (N63050.114' E38025.003' - N63050.338' E38024.948'). Sampling points belonged to autonomous, transitional and subordinate types of terrain.

Analysis of heavy metals concentration in samples was carried out by ICP-OES method using Shimadzu ICPE-9000 instrument, after microwave digestion with HNO3 using Analytic Jena TopWave system. Construction of elements spatial distribution maps is performed using "Surfer" software (Fig. 1).
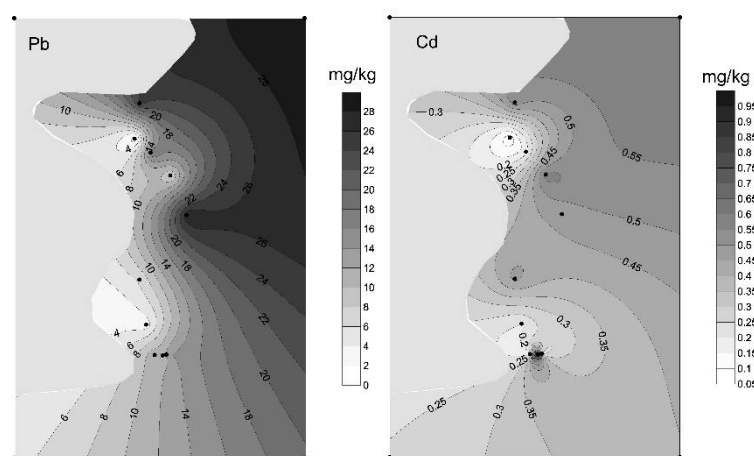
Figure 1 - Spatial distribution of Pb and Cd in soils

The highest concentrations of heavy metals are related to subordinate terrain, while autonomous landscapes are characterized by a minimum content of Pb and Cd.

In this way, it was shown that upper horizon of podzolic soil of northern taiga is characterized by evaluation of elements from autonomic terrain into subordinate with groundwater runoff, which should be taken into account in determining the regional background concentrations and in assessing the negative impact on soil cover.

(P-28)

ANALYSIS OF TRACE ELEMENTS DISRIBUTION BY BIOLOGICAL PATHWAYS ON THE TERRITORY OF EUROPEAN RUSSIA ARCTIC USING ICP-MS TECHNIQUE

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Trace elements are persistent ecotoxicants, that can accumulate in food chains and spread transboundary by biological pathways. The transmission of this pollutants significantly provided by migratory animals, especially birds and fish. Fish is one of the main sources of nutrition for the indigenous people of the Russian Arctic and Subarctic. Therefore, accumulated by fish trace elements may penetrate the human body through the traditional nutrition. For this reason, sampling of fish from the indigenous people fishing areas and its further analysis can provide an information on the distribution and transmission of pollutants on the Arctic territories, and its impact on human health.

Fish sampling was performed during the expedition of the Arctic floating university provided by the Northern Arctic Federal University (NArFU) and expeditions to the Nenets Autonomous Region on the shore of White and Barents seas and the estuary of Pechora river. Fish samples were collected by the local fisherman and are a typical nutrition of the Nenets Autonomous region indigenous people. Freshwater species: whitefish Coregonus lavaretus, perch Perca fluviatilis and pike Esox lucius as well as marine species: Salmon Salmo salar, navaga Gadus navaga Kolreuter and Cod Gadus morhua were homogenized and then treated by microwave digestion procedure and estimated on AAS AA-7000 Shimadzu (Japan) and ICP-MS Bruker Aurora Elite (USA) for Hg, Cd, Pb.

The highest for this study content of pollutants was found in sea water predators with spikes of Cd and Pb in 4 Cod samples at the concentration levels ~ 0.5 mg/kg Pb and ~ 0.1 mg/kg Cd. Spike of ~0.05 mg/kg Hg was found in navaga. The remaining samples are characterized by the background value of heavy metals at the ppb concentration level.

(P-29)

DETERMINATION OF ELECTRON TEMPERATURE AND CONCENTRATION IN CADMIUM AND ZINC CONTAINING HIGH-FREQUENCY ELECTRODELESS LAMPS

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Multi-element light sources, like high-frequency electrodeless lamps (HFEDL) filled with two working elements, provide unique possibility to determine concentrations of several elements simultaneously; furthermore, they can be of interest also in spectroscopic diagnostics of plasma due to the possibility to study interactions between working elements. Such investigations are important to understand the processes inside the plasma, thus it helps in optimization process of the light sources.

In this study for determination of electron temperature and concentration in HFEDLs we use approach based on assumption of local thermodynamic equilibrium. In such case Saha equation describes the relation between electron temperature (T_e), the ionic and atomic line ratio (involving excitation temperature T_{exc} via Boltzmann function) and electron concentration. In literature it is also possible to find the modified Saha equation which takes into account gas temperature (different from electron temperature) as well.
Saha equation allows determining either electron temperature or concentration if other one is known (for instance, obtained with different method).

The light sources under study were high-frequency electrodeless lamps filled with cadmium and zinc (with argon as buffer gas): (1) Zn+Cd+Ar (p = 3 Torr) and (2) Zn+Cd+SbI$_3$+Ar (p = 2,7 Torr). HFEDLs consist of spherical part (with diameter of 1cm) and small side-arm. The discharge is ignited at the spherical part of the lamp by placing it into the electromagnetic field of 100 MHz frequency. The emission from lamps was registered using JobinYvon SPEX 1000M spectrometer for different excitation generator voltages (21V – 29V).

In this study electron temperature was determined with modified Boltzmann plot method using emission spectra of argon atom, and the electron-impact excitation coefficients were used in modified Arrhenius form. The excitation temperature was obtained from the relative intensities of argon atomic spectral lines, too. For both HFEDLs it was obtained that excitation temperature just slightly differs from the determined electron temperature (T_e ~ 0.6 eV and T_{exc} ~0.5 eV). The determined electron concentration for both lamps was around $10^{12} – 10^{13}$ m^{-3}. Since the lamps contain Zn and Cd, ionic and atomic lines of both elements were used to estimate the electron concentration, and both showed similar results.

(P-30)

DETERMINATION OF VIBRATIONAL TEMPERATURE OF CN MOLECULE IN THALLIUM CONTAINING HIGH-FREQUENCY ELECTRODELESS LAMPS

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High-frequency electrodeless lamps (HFEDL) are known to be very convenient light sources for use in atomic absorption spectrometers. They provide good detection limits for concentration determination of numerous elements, like, mercury, cadmium, zinc, thallium etc. For each particular use, the HFEDLs need to undergo the optimization procedure in order to find the best amount of working element, best working regime and so on. To successfully achieve the goal, it is very important to understand the processes inside the plasma and to obtain information about different plasma parameters, for instance, different temperatures.

Usually the HFEDLs are filled with working element (one or several) and buffer gas, so the emission spectrum should contain only emission from these filled in elements, however, in some cases we can also register the emission of OH, CN, N_2, C_2 and other complexes. These molecules are considered to be impurities, but they can also be used to obtain different plasma parameters. For determination of gas temperature it is common to use emission of OH at 306.4 nm and C_2 at 516 nm (rotational temperature of these molecules can be considered to be equal to gas temperature). The emission spectra of these molecules can also provide the information about vibrational temperature.

In this study we focus our attention on determination of vibrational temperature of CN molecule in thallium containing HFEDLs. The plasma under study are $Tl^{205}I+Ar$ (3 Torr) and $Tl^{205}+SbI_3+Ar$ (2.6 Torr) HFEDLs. The discharge is excited using electromagnetic field with frequency of 100 MHz. The voltage of excitation generator varies in range from 21 V to 29 V. Emission spectra are registered using high-resolution spectrometer JobinYvon SPEX 1000M with diffraction grating 1200 mm^{-1}.

In spectra of lamps of both types it is possible to identify presence of OH and CN, and in $Tl^{205}+Ar$ HFEDL also C_2. Gas temperature estimated using OH for both lamps was slightly less than 1000 K. The Rotational temperature of C_2 was for about 400K higher (as we have observed it in our previous measurements). The vibrational temperature of $Tl^{205}I+Ar$ HFEDL is estimated to be around 9000 K, and the HFEDL with addition of SbI_3 ($Tl^{205}+SbI_3+Ar$) has vibrational temperature of CN higher, being ~ 11000 K. This difference can be explained by the differences in filling, namely, the higher vibrational temperature of $Tl^{205}+SbI_3+Ar$ HFEDL is due to addition of Sb, which combines with excess of iodine thus minimizing the quenching effect of iodine.

(P-31)

DETERMINATION OF ARSENOLIPIDS IN BREAST MILK BY HPLC-ICPMS AND HPLC-ESMS

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Recent research1,2 has shown that some arsenic containing lipids, common components of seafood, are highly cytotoxic and have the potential to cross the blood-brain barrier. Infants, in particular, are especially sensitive to exposure. Thus the aim was to identify and quantify arsenic containing lipids in breast milk from the Norwegian Human Milk Study (HUMISNoMIC), a prospective population-based birth cohort consisting of over 2500 mother-child pairs established with the purpose of studying environmental toxicants in human milk and their relation to children's health. Initial testing of 10 milk samples had shown that a significant proportion of the total arsenic occurred in lipid-soluble forms, and identified the major arsenolipids in 5 of those samples3. In the present work, 21 additional breast milk samples were processed and analysed with high performance liquid chromatography coupled through a splitter to elemental and molecular mass spectrometers to determine both molecular structures and concentrations of the arsenolipids. The concentrations of arsenolipids in the human breast milk samples were low (<1,0 μg As/kg), but could still be of concern considering the sensitivity of the developing brain to toxicants and the neurotoxicological potential of arsenolipids.

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(P-32)

ARSENIC, BROMINE, AND LEAD IN BREAST MILK AND URINE FROM NORWEGIAN MOTHERS – INTERACTIONS WHICH INFLUENCE THE LEVELS

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Norwegian health authorities recommend that breast milk is given exclusively for the first six months of the child's life. Through breast milk, the child's need for vitamins (except vitamin D), minerals and nutrients are covered, provided the mother has covered all her nutritional needs Breast milk is the ideal food for optimal growth, health and development of infants, but it is also a source of environmental pollutants. Due to rapid growth, immature kidney and liver, and nervous system under development, infants are especially sensitive to toxic elements compared with older children and adults. Thus, knowledge on the presence and level of both essential and potential harmful elements in breast milk is important to increase public awareness.

Five Health Centers in Oslo were randomly selected during 2016, and 175 lactating women between 2nd and 28th weeks postpartum were recruited, all women with a mean age of 32 years (range 23-44). Thirty-five percentage of the women were born in another European country, in Asia, Africa, or South-America; however, all immigrants have lived in Norway the last 1-31 years (median 7 years). Each woman was asked to give four portions of breast milk, two in the morning just after eating breakfast, and two in the afternoon; two with foremilk and two with hind milk. A spot urine sample was obtained in the morning, shortly after breastfeeding the baby. The breast milk and the urine were analyzed using triple quadrupole inductively coupled plasma mass spectrometry (ICPMS-QQQ). The samples were prepared by dilution with an alkaline solution (BENT) containing 1-butanol, H_4EDTA, NH_4OH and Triton™, X-100. The participants replied to a questionnaire on background information, habitual intake of 31 food items, in addition to intake of dietary supplements. Multivariate linear regression was used to examine predictors of arsenic (As), bromine (Br), and lead (Pb) in the breastmilk and the urine. In particular, a significant positive association ($p<0.001$) between consumption of fish and As in breast milk was noticed. Results showed that the median concentrations of As and Pb in breast milk, and Pb in urine are among the lowest reported in Europe (Björklund *et al.* 2012; Eik 2016; Krachler *et al.* 1998; Leotisindis *et al.* 2005; Vollset, 2015). However, the total concentration of As, Br, and Pb in breast milk and urine showed considerable individual variations.

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(P-33)

ANALYSIS OF SILVER NANOPARTICLES IN MUNICIPAL WASTEWATER SLUDGE USING SP-ICP-MS

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Exponential growth in use and applications of nanotechnology has increased awareness of nanoparticles released into the environment. One of the sinks of nanoparticles is municipal wastewater sludge, which is produced in vast quantities in wastewater treatment plants all around the world. Concentrations of heavy metals in sludge are well documented, but there is still little knowledge on nanoparticle concentrations in sludge. One of the most interesting elements present in the environment as nanoparticle form is silver, due to its potency to cause adverse effects on living organisms. Due to the common use of wastewater sludge as fertilizer in agriculture, analysis of potentially harmful nanoparticles in sludge is of great importance.

Single particle ICP-MS has emerged more than ten years ago as a technique capable of analyzing single nanoparticles in liquid suspensions. The recent advances in spICP-MS have made it possible to analyze concentration, size distribution, and even composition of nanoparticles in environmental matrices. However, challenges in sample pretreatment and determination of transport efficiency, for example, have shown the need for more research in order to make spICP-MS a reliable and reproducible instrument in the analysis of nanoparticles.

In this study, silver nanoparticles (AgNPs) were analyzed using spICP-MS from municipal wastewater sludge collected from a treatment facility in central Finland. Several parameters in the sample pretreatment and analysis stages were studied, and were found to have effects on the final results, especially on AgNP concentration. The studied factors were: storage conditions of sludge, solid to liquid ratio in leaching, leaching agent, separation of solid from liquid, dilution factor, and method for determination of transport efficiency. Both natural sludge samples and AgNP spiked sludge samples were analyzed to evaluate the recovery and transport of AgNPs during pretreatment and analysis.

All the studied parameters had major effects on concentration of AgNPs, but effects on nanoparticle size were not as pronounced. Determination of particle size distribution with spICP-MS was found more reproducible than determination of particle concentration, which was easily affected by several parameters in the sample pretreatment and analysis stages of wastewater sludge.

(P-34)

DETERMINATION OF HEAVY METALS IN POST-PRECIPITATED SEWAGE SLUDGE BY ICP-MS

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It is well known that during wastewater treatment heavy metals end up in the sewage sludge along with phosphorus. This does not only restrict the agricultural use of the sludge, but also presents a challenge for processing the sludge further for phosphorus recovery.

The problem can be overcome with chemical post-precipitation of phosphorus, where phosphorus is precipitated at the end of wastewater treatment process. This should yield a sludge fraction with low heavy metal content, which can then be further processed for phosphorus recovery. In this study, the heavy metal content of post-precipitated sewage sludge was analyzed. The sludge was acquired from a pilot plant located in wastewater treatment plant in southern Finland. It was dried at 105 °C for 16 hours and then manually ground in a mortar. The samples of 200 mg were microwave-digested. The digestion was done according to the EPA 3052 method. The heavy metals analyzed were As, Cd, Cr, Ni, Pb, Sb, Se, Sn, Te and Zn. The element concentrations were determined with a PerkinElmer NexION 350D inductively coupled plasma mass spectrometer and the obtained results were compared to to the literature values of conventionally precipitated sewage sludge.

(P-35)

SELECTIVE RECOVERY OF RUBIDIUM USING 3D-PRINTED POTASSIUM COPPER HEXACYANOFERRATE FUNCTIONAL FILTERS

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Valuable rubidium has high abundance in the earth's crust, but it is usually widely spread and not found in high concentrations in any minerals. Rubidium can concentrate in fly ash when wood, beat or coal is used are used as fuel in industrial combustion process. This makes fly ash a useful source for recovery of rubidium.

Potassium metal hexacyanoferrates have been used for removal on radioactive cesium in nuclear waste brine, and recently, the same method has been adapted for extraction of rubidium using polymer encapsulated copper based potassium hexacyanoferrates ($K_2[CuFe(CN)_6]$).
In the present study, 3D-printed nylon based potassium copper(II) hexacyanoferrate functional filters have been employed for selective recovery of rubidium from synthetic samples mimicking acid leached fly ash. 3D-printed functional filters selectively absorbed up to 95% of rubidium from high matrix samples. Different concentrations sodium nitrate solutions were used for desorbing rubidium from the filters resulting in high recovery of rubidium and low concentrations of matrix elements.

3D-printed potassium copper hexacyanoferrate functional filters can be a simple, effective and fast tool for selective recovery of rubidium from leached industrial fly ash and possibly other materials.

(P-36)

DEPARTURE FROM THERMODYNAMIC EQUILIBRIUM IN THERMAL PLASMA ARCJET, EMISSION SPECTROSCOPY STUDY

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Thermal plasmas are widely used in various industrial applications, namely plasma spraying, waste treatment, plasma cutting and others. In Institute of Plasma Physics in Prague, so called water-stabilized plasma torch has been developed. Its gradual evolution led to currently used hybrid water-argon torch. This torch has been successfully applied especially for plasma spraying and for waste treatment and gasification of organic substances. Nowadays its investigation continues mainly in connection with these applications. Several reactors are installed in IPP for this purpose. In such a reactor, usually controlled atmosphere is formed, in order to fulfill requirements of the certain application. Also the reactor chamber pressure is often varied in a reasonable extent. Then we often encounter situations, in which departures from local thermodynamic equilibrium (LTE) appear. On the other hand, operation of thermal plasmas in atmospheric pressure can be usually described by equilibrium relations.

This contribution deals with several aspects of equilibrium and non-equilibrium behavior in plasmas generated in above-mentioned water-argon plasma torch. We study these plasmas in atmospheric pressure as well as in controlled atmosphere with pressures between 500 Pa and 100 kPa. Emission spectroscopy and high-speed camera diagnostics are used. The torch operates in continuous direct current mode; however, temporally resolved measurements in the order of tens of microseconds reveal that during operation of the torch periodical patterns are present. Optical arrangement allows reaching spatial resolution in the order of millimeters. Altogether, we obtain spectrally, temporally and spatially resolved characterization of the plasma.

We are going to present results of measurement for reactor pressures 2, 4, 10 and 20 kPa. Continuous supply of water-argon plasma makes the atmosphere in the reactor composed mainly of steam with argon admixture. The study includes analysis of large number of emission spectral lines. From the hydrogen Hβ line we are able to obtain electron density distribution in the plasma. This brings first insight into the non-equilibrium phenomena, by means of application of Griem's or McWhirter's criteria. We also analyze other lines of hydrogen Balmer series, and lines of atomic and singly ionized argon and oxygen. In addition emission spectra of OH and NH radicals are measured, the latter one in case of additional nitrogen supply into the chamber. Using all these lines, Boltzmann plots are constructed and further details regarding departures from LTE are obtained. In case of temporally resolved spectra, fast processes influencing the equilibrium are studied.

(P-37)

A FIRST COMPREHENSIVE STUDY ON ZINC ISOTOPIC VARIATION OF WATER AND SURFACE SEDIMENT SAMPLES FROM THE ELBE RIVER

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Zinc is one of the most important metals for industrial applications and therefore an important anthropogenic contaminant affecting the environment. Whereas the usage of Zn isotopic analysis as a tracer for anthropogenic emissions was highlighted in the past decade, only few examples on the application of such analysis for the investigation of river and coastal environments exist so far.

Our contribution will address this issue by analyzing sample sets of water and surface sediment from various locations within one of Europe's largest rivers, the Elbe. For decades, the Elbe was considered one of the most contaminated European rivers. In this study, 19 water and 26 surface sediment samples were analyzed for Zn concentration and Zn isotopic composition by inductively coupled plasma tandem mass spectrometry (ICP-MS/MS) and by multi collector inductively coupled plasma mass spectrometry (MC ICP-MS), respectively. The analyzed samples covered the complete course of over 700 km of the German Elbe between the German/Czech border and the German North Sea. Additional samples were taken in 6 different tributaries (e.g. Havel, Saale and Mulde). Zn isotope ratios were assessed in water filtrates (<0.45 µm) or total digests of the surface sediment fraction (<63 µm) after analyte/matrix separation using Bio-Rad AG MP-1 resin via a micro-column approach and application of a $^{64}Zn/^{67}Zn$ double spike.

The adapted micro-column extraction approach enabled quantitative recovery of Zn for both water and sediment samples (recoveries of 88% to 113%) as well as procedural blanks of 1.0 ng ± 0.2 ng (*n*=6). Measurements of the IRMM-3702 reference material resulted in an external precision of $\delta(^{66}Zn/^{64}Zn)_{IRMM-3702}$: -0.02 ± 0.10 (*k*=1, *n*=22). Measured isotopic compositions of $\delta(^{66}Zn/^{64}Zn)_{IRMM-3702}$ ranged from -0.1 to 0.3 for sediment samples and from -0.5 to 1.4 for water samples. Zn concentrations varied from 42 mg kg^{-1} to 1120 mg kg^{-1} for sediment samples and 4.3 µg L^{-1} to 1697 µg L^{-1} for water samples.

Our studies revealed distinct changes in isotopic composition and Zn concentration particularly for water and sediment samples taken in different tributaries of the Elbe. Elevated Zn concentrations were found at several sampling locations which were consistent with samples analyzed during the 1990s by Prange *et.al*. Our results highlight the suitability of Zn isotope analysis, as a potential tracer for anthropogenic emissions of Zn into the aquatic environment.

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DETERMINATION OF ELEMENT PROFILES IN ATLANTIC SALMON SCALES BY LA-ICP-MS

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As the number of farmed Atlantic salmon rises and the wild population declines, farm escapes have become a major ecological problem in Norway. Escapees compete with wild salmon for food and breeding grounds while decreasing the genetic variation in the native population. Recently, the Norwegian salmon industry has developed a tracking system for escaped fish.

As part of the tracking system, element profiles in salmon scales are used to distinguish between groups of fish. These profiles are a result of the geological variation found throughout Norway, which affects element concentrations in waters and thus elements incorporated in the outer, hydroxyapatite (HAP) layer of salmon scales. This outer layer grows like the rings of a tree, creating a timeline of exposure to different water environments, like the transition from fresh water to seawater. Different regions of the scale can be sampled: the innermost freshwater region, the outermost seawater region, and/or across the entire scale from center to edge.

Analysis of this HAP layer is carried out using an HR-SF-ICP-MS (Element 2, Thermo Fisher Scientific) connected to an excimer 193 nm laser (New Wave Research, ESI).
The isotopes measured are ^{7}Li, ^{11}B, ^{137}Ba, ^{208}Pb, and ^{238}U in low resolution (m/Δm = 300) and ^{23}Na, ^{24}Mg, ^{32}S, ^{52}Cr, ^{55}Mn, ^{56}Fe, ^{66}Zn, and ^{88}Sr in medium resolution (m/Δm $\approx$ 4000). ^{42}Ca is measured in both resolutions as an internal standard, using the previously reported value of 37.4 $\pm$ 0.4% Ca in the hydroxyapatite layer of salmon scales (Flem et al. 2017). Results are externally calibrated using NIST SRM 610, 612, 614 as well as two custom-made apatite standards (Avantama AG). Reference scales from fish farms are collected and analyzed to provide group elemental profiles to which scales of unknown origins can be matched using multivariate statistics and classification models.

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(P-39)

QUANTITATIVE ANALYSIS OF INORGANIC ARSENIC IN FOOD AND FOOD PACKAGING USING LC-ICP-MS

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Food safety is one of the major concerns of the European population and the European Commission is aiming to assure a high level of food safety and animal & plant health within the EU through the farm-to-fork principle. This implements effective control systems for harmful substances such as pesticides, mycotoxins and heavy metals.

Nowadays in food control the speciation analysis has become an important tool for the determination of elements like lead, cadmium, mercury, tin, and arsenic where simply the measurement of the total amount of the element is not sufficient.

The idea is to have a clear identification and quantification of the different species for a better understanding of toxicological impacts on human health, animal health and the environment.
Hot subject discussions are recently on the concentration levels of mercury in fish, as Mercury and most of its compounds are extremely toxic and must be handled with care. Most toxic however is the organic species of mercury, the methylmercury with a tolerable weekly intake of 1.6 µg/Kg body weight.

In contrast the inorganic arsenic species arsenite and arsenate have a bigger toxicological relevance than the organic species. Both organic and inorganic arsenic species occur naturally. The organic arsenic, which can be found in seafood, is not known to be harmful, but inorganic arsenic, which enters plants through water and soil, is toxic. Long-term exposure can cause cancer and has also been linked with cardiovascular disease, neurotoxicity, and diabetes. The European commission has fixed the maximum levels of inorganic arsenic in Non-parboiled milled rice at 0.2 µg/Kg and rice for the production of food for infants and young children at 0.1 µg/Kg [1].

The Shimadzu LC-ICP-MS system which connects an inductively coupled plasma mass spectrometer (ICP-MS) in-line with a high-performance liquid chromatography (HPLC) system allows the high sensitive and high accuracy measurement of arsenic species in foodstuff. Analytical data are presented and advantages of the system configuration will be explained.

[1] COMMISSION REGULATION (EU) 2015/1006, 25 June 2015, amending Regulation (EC) No 1881/2006 as regards maximum levels of inorganic arsenic in foodstuffs

(P-40)

TOWARDS A FUTURE SCREENING METHOD FOR NANOPARTICLES IN SEAFOOD -FOR SURVEILANCE AND RISK ASSESSMENT OF FOOD SAFETY

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Nanoparticles are produced or engineered, intentionally, due to their product improving properties. However, nanoparticles are also produced unintentionally, for example in mining and abrasion processes. Nanoparticles have a large surface area to volume ratio, which implies a different behavior of the compounds compared to larger particles or single ions/molecules of the same compound. Therefore, the compounds are more reactive per weight unit than larger structures of the same compounds and have different toxicities and risks compared to single ions or molecules of the same element. Negative effects of manufactured NPs on organisms, including invertebrates, fish and mammals, have been demonstrated, and the release of NPs in the marine environment may therefore cause negative effects in marine organisms. The new analytical dimension of size thus needs to be added to the already established total and species specific determination of metals and elements to aid in the future risk assessments of food safety.

This work focus on the development of a generic analytical screening method for metal containing nanoparticles (NPs) in seafood using single particle inductively coupled plasma mass spectrometry (sp-ICP-MS). Challenges in calibration, standards and reference materials for different elements will be discussed using both the particle size and particle frequency method. Sample preparation based on different protocols, such as liquid extraction and enzymatic digestion will be compared for selected matrixes.

Our future objective is to be able to evaluate the effect of deposits of mining waste in Norwegian fjords on seafood safety. Mining waste contains a high fraction of fine particles, including particles with sizes in the nano-meter range. Complementary techniques such as transmission electron microscopy (TEM) and asymmetric flow field flow fractionation (AF4) will be needed to obtain more specific information on the nanoparticles analysed by sp-ICP-MS.

(P-41)

AUTOMATED, HIGH-VOLUME PRECONCENTRATION AND MATRIX REMOVAL SYSTEM FOR ULTRATRACE QUANTIFICATION AND ISOTOPIC DETERMINATION OF TRACE ELEMENTS IN SEAWATER

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The study of stable isotopes of bioactive trace elements in seawater is a relatively new field of marine chemistry providing insights into marine cycling of these elements. Due to the small variation found in isotope ratios, large volumes of seawater must be preconcentrated to successfully determine differences in ratios for trace elements, making it impractical to process a large number of samples. Furthermore, manual preconcentration techniques have many steps that may introduce contamination and degrade the analytical quality of the determination, making it necessary to further increase sample size. By automating the preconcentration and matrix removal process, blanks are minimized and the required sample volume is decreased, allowing higher throughput sampling and analysis. A new system for automatic preconcentration and matrix removal of large-volume samples (>1 L) is presented which minimizes blanks, increases throughput, and enables routine processing of marine samples for ultratrace quantification and isotopic determination of trace elements in seawater.

(P-42)

PERFORMANCE DATA FOR A NEW MULTI-COLLECTOR ICP-MS WITH A MULTI-POLE COLLISION CELL INTERFERENCE REMOVAL DEVICE

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Multi-collector ICP-MS (MC-ICP-MS) has been used for 20 years with little change to the basic configuration of a forward geometry magnetic sector ICP-MS with an array of faraday and ion counting detectors used to simultaneously collect the signals from multiple ions over a narrow mass range. Whilst the ICP is a powerful ion source capable of reducing virtually all matrices to individual ions, it also has several well-characterised issues with overlapping ion signals from polyatomic ion species at the same masses as some of the isotopes of interest for key elements. In the field of quadrupole ICP-MS, the collision or reaction cell has now become a near essential requirement as the quadrupole does not offer the option to resolve interferences. With the exception of the GV Isoprobe, which is no longer available, no commercially available MC-ICP-MS has used a collision cell.

A new multi-collector ICP-MS with a collision cell, Nu Sapphire, is presented with the characteristic performance data for a range of key isotope groups. Data will be shown to prove the performance of the novel MC-ICP-MS design with a dual ion path. The ion-beam from the ICP interface can be directed either through an RF multipole collision cell or by-passing the cell direct to the mass analyser to operate as a conventional MC-ICP-MS. Both collision cell and conventional data will be shown along with comparison of the same tests on current technology Plasma 3 instruments.
Performance for classically difficult elements such as potassium and calcium will be shown.

(P-43)

IMPROVED IN-SITU Δ⁷LI ANALYSIS OF SYNTHETIC GLASS BY LA-MC-ICP-MS WITH 1013 Ω AMPLIFIER TECHNOLOGY

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The application of 1013 Ω amplifier technology to lithium isotope ratio analysis by LA-MC-ICP-MS is demonstrated to improve precision at typical lithium concentrations for geological materials. The Thermo Scientific™ NEPTUNE Plus™ MC-ICP-MS was coupled to a Teledyne™ Photon Machines™ Analyte G2™ excimer laser with 193 nm wavelength. The laser was equipped with a HelEx™ II two-volume ablation cell. Li isotope ratio analysis ($^7Li/^6Li$) was performed on six synthetic MPI-DING glasses (T1-G, ATHO-G, GOR132-G, StHs/680-G, KL2-G and ML3B-G). A seventh MPI-DING glass, GOR128-G was used as the external standard. 5 individual spot ablations were made on each glass, bracketed by 2 spots on the external standard. A 60 s on-peak baselines was measured between each ablation. The analysis was performed twice, once with 1011 Ω and once with 1013 Ω amplifiers.

The measured ^6Li sample signal ranged from 2.1 – 13 mV and was 5.3 mV for the external standard GOR-128-G (Li concentration 10.4 ppm). The baseline was approximately 200 μV for ^6Li. For all six MPI-DING glasses using the 1013 Ω amplifiers resulted in significant improvements in both internal and external precision. KL2-G and ML3B-G, with the lowest concentrations of ^7Li, observed a four to fivefold reduction in both internal and external 2SD. At 28.0 – 30.4 ppm ATHO-G had the highest concentration of the MPI-DING. Even at this elevated concentration and signal the 1013 Ω amplifiers resulted in at least a threefold improvement in precision.

Using the better $^7Li/^6Li$ precision achieved with the 1013 Ω amplifiers, the two Komatiite glasses, GOR128-G and GOR132-G, could be distinguished from each other. StHs6/80-G and ATHO-G could now also be identified as having different Li isotopic compositions by using 1013 Ω amplifier technology.

For the smallest intensity ion beams, KL2-G and ML3B-G, using the 1013 Ω amplifier introduced a large shift (≈ 5‰) in the measured mean δ⁷Li value (Table 2; Figure 2). Smaller shifts were detected with T1-G and GOR132-G. It was concluded that the high uncertainty at low count rates with the 1011 Ω amplifiers introduced a positive bias to the measured ^6Li signals and therefore changing the calculated mean ratio.

Due to the low abundance of Li in geological materials, more precise δ⁷Li values can be obtain for LA-MC-ICP-MS by employing 1013 Ω amplifiers. The ±0.31‰ (Ext 2SD) external precision achieved for MPI-DING silicate glass ATHO-G represents an approximately fourfold improvement over both the 1011 Ω amplifiers (±1.37‰) and published values (±1.2‰) 3. Similar enhancements in precision were observed for all the MPI-DING glasses.

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