LOEWE-Schwerpunkt AmbiProbe

Vollantrag auf Einrichtung eines LOEWE-Schwerpunktes an der Justus-Liebig-Universität Gießen (Federführung)

„AmbiProbe – Massenspektrometrische *in-situ*-Analytik für die Problembereiche Gesundheit, Umwelt, Klima und Sicherheit“

Projekt A.1: Development of novel ionization techniques for in-situ detection

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Summary

Objectives: Developing novel, robust ionization methods and ion sources which are capable of directly converting constituents of biological samples into corresponding gaseous ions.
Methods: We plan to further develop the recently developed Jet-Desorption Ionization and Rapid Evaporative Ionization Mass Spectrometry techniques.
Innovative Aspect:
Two new ionization techniques
Direct, in some cases in-vivo investigation of biological samples
Relation to other Schwerpunkt-Projekten:
Ion sources for instruments developed in projects C1-C3

Intoduction

Mass spectrometric methods traditionally involve multi-step sample preparation procedures, including homogenization of sample, extraction, solvent exchange, gas or liquid chromatographic separation of analytes prior to actual mass spectrometric detection. This fact, together with the size, weight and delicateness of mass spectrometric instrumentation has hindered the routine field application of mass spectrometric methods. On the other hand, various fields from forensics through food safety, to cancer surgery would need real-time, in-situ chemical analysis with no compromise on the reliability of analytical results. The recent development of ambient or direct ionization techniques has opened the door to the development of mass spectrometric instrumentation for these application fields.

Objectives

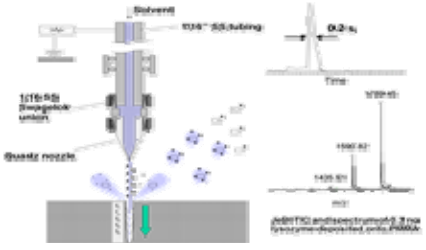
The main objective of the project is to develop robust ion sources for portable mass spectrometric instrumentation. Novel Ion sources will allow the mass spectrometric analysis of various samples within timeframe of a few seconds. Since the fast, in-situ analysis cannot involve elaborate sample preparation, the ionization methods will presumably work with no or minimal sample preparation procedure.
Project is focused on the qualitative/semi-quantitative determination of mainly low molecular weight compounds in biological matrices. Analytes include metabolic constituents, xenobiotics, drugs, or drug candidate molecules, structural lipids, hormones and microbial markers.
Primarily we plan to utilize and further develop techniques termed Jet Desorption Ionization and Rapid Evaporative Mass Spectrometry, however application of Desorption Electrospray Ionization and Desorption Atmospheric Pressure Chemical ionization is also planned.

Methods

We plan to build robust ion sources utilizing primarily Jet Desorption Ionization (JeDI) and Rapid Evaporative Ionization Mass Spectrometry (REIMS).
JeDI technique is implemented by directing a contimuous water jet onto surface of sample. On the impact of water jet, aueous droplets are formed, which contain dissolved analyte molecules. Charged droplets undergo electrospray-like process and eventually produce gaseous ions of analyte molecules. Charging of droplets occurs spontaneously (cf. sonic spray ionization), however application of electric field gradient between sample and inlet of mass spectrometer enhances ionization efficiency by several orders of magnitude.
Rapid Evaporative Ionization Mass Spectrometry utilizes gas phase ion formation occuring on the rapid thermal evaporation of ionic solutions or solid samples containing large amounts of ionic solutions. Thermal evaporation is implemented by using contact heating, Joule-heating, dielectric heating, or laser heating. The technique can be combined with secondary electrospray ionization to enhance ionization efficiency.

Preliminary results

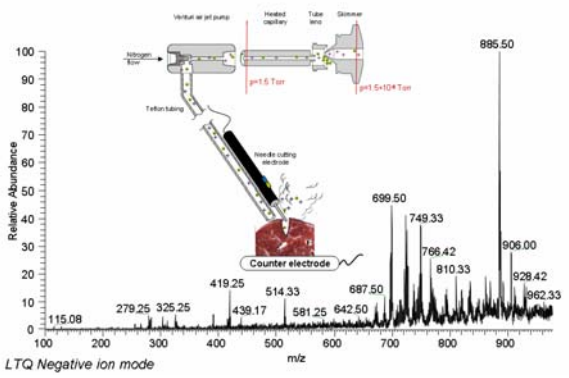
Jet Desorption Ionization was already implemented and tested at various applications. As figure shows, spectral characteristics of JeDI is similar to that of Electrospray Ionization. In comparison with Desorption Electrospray Ionization, JeDI offers higher spatial resolution, more mechanical invasiveness, and higher overall ion yield. Since the ion source does not utilize high amount of nitrogen, and does not necessarily contain thin capillaries, the technique suits better field applications than DESI.



Rapid Evaporative Ionization has been first implemented recently. The mechanism of technique has been studied, and found to be similar to IR-MALDI of aqueous solutions and Thermospray ionization. Surgical applications of technique have been explored, since number of surgical techniques were found to produce tissue-originated gaseous ions following the same mechanism. Tissue identification system was created and fundamentals for mass spectrometry-guided surgery were laid down.

Work plan

Arbeitspaket 1: Entwicklung einer miniaturisierten gepulsten Mikrowellenheizung, sowie einer Sonde mit Ionentransferkanal. Kopplung mit Transfereinheit aus Projekt B1.
Arbeitspaket 2: Entwicklung einer JeDI-Ionenquelle und Sonde mit Ionentransferkanal. Kopplung mit Transfereinheit aus Projekt B1.
Arbeitspaket 3: Charakterisierung der Ionenquellen hinsichtlich relevanter Eigenschaften, wie Nachweisgrenze, zugängliche Substanzklassen, Fragmentierungsgrad.
Arbeitspaket 4: Anwendung auf realistische Testprobleme in Gewebe oder typischen Materialien.



Literature

1. Cooks, RG; Ouyang, Z; Takats, Z; Wiseman, JM. 2006. Ambient mass spectrometry. SCIENCE 311 (5767):1566-1570, .
2. Takats, Z; Wiseman, JM; Cooks, RG. 2005. Ambient mass spectrometry using desorption electrospray ionization (DESI): instrumentation, mechanisms and applications in forensics, chemistry, and biology. JOURNAL OF MASS SPECTROMETRY 40 (10):1261-1275
3. Takats, Z; Wiseman, JM; Gologan, B; Cooks, RG. 2004. Mass spectrometry sampling under ambient conditions with desorption electrospray ionization. SCIENCE 306 (5695):471-473,

Arbeitsplan	1. Jahr				2. Jahr				3. Jahr			
A1 - REIMS/JeDI												
Entwicklung Mikrowellenheizung und Sonde												
Entwicklung JeDI-Ionenquelle und Sonde												
Charakterisierung Ionenquellen												
Anwendung auf Testsysteme												