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Further Development and Optimization of a Successfully Implemented Accumulation Ion Source

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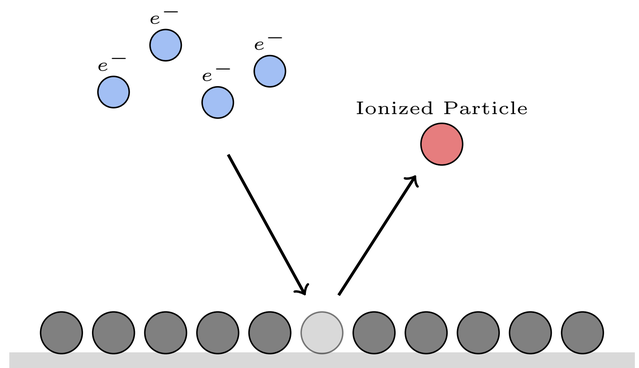
Introduction

- The enrichment of analytes is a widely employed technique for the detection of molecules at partial pressures below the detection limit of electron ionization (EI).
- Mass spectrometry (MS) at ultra-trace levels requires optimized sampling and acquisition systems, capable of measuring gaseous metal hydrides with maximum sensitivity.
- The presence of these metallic fragments has been observed on surfaces.
- In a plasma chamber, metal hydride fragments form when metal interacts with ionized gases.
- Such fragments readily decompose on EI source walls and subsequently desorb from the surfaces due to electron-induced desorption.

Fig.1: (on the right) illustrates the electron-induced desorption mechanism.



Geometry of the Source

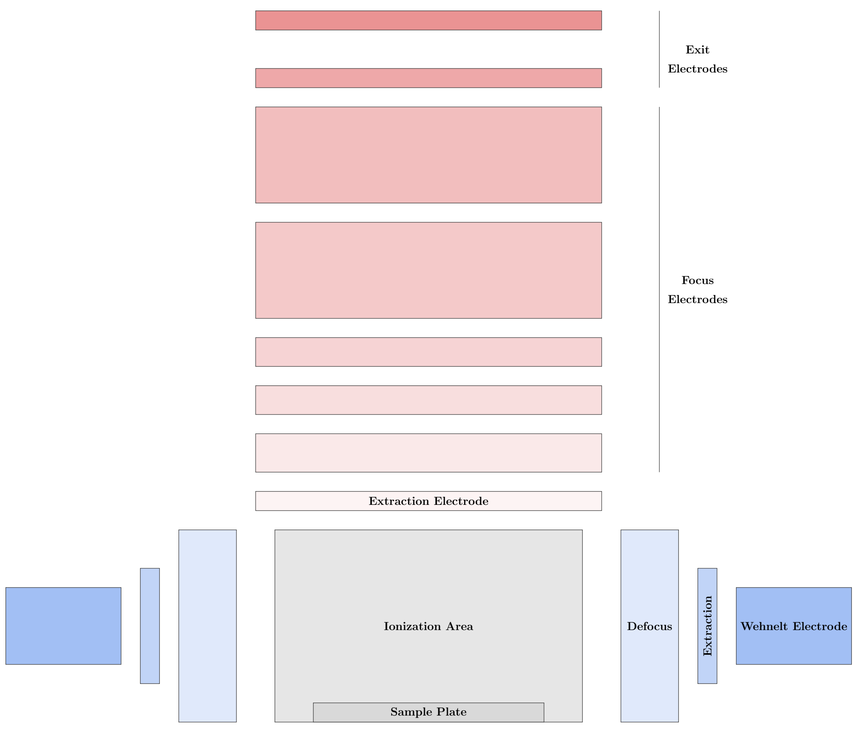


Fig.2: Geometry of the ion source.

- The ion source is designed for the purpose of sample accumulation, with a probe inserted in-situ into a plasma chamber.
- Following the enrichment of the analytes on the heated metal surface, the probe is transferred back into the ion source with a linear actuator. The ion source is positioned directly in front of the ion optics of a cTOF MS[2].
- Two filaments positioned adjacent to the sample, each equipped with a lens system, generating an electron beam directed towards the probe surface.
- A further lens system guides generated ions into the quadrupole and the mass analyzer.
- Exit electrode potential allows a variation of the kinetic energy.

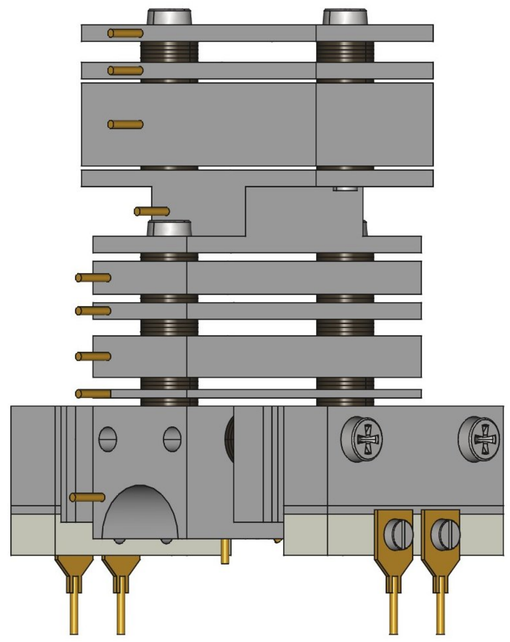


Fig. 3: CAD Model of the novel ion source.

Simulated Trajectories

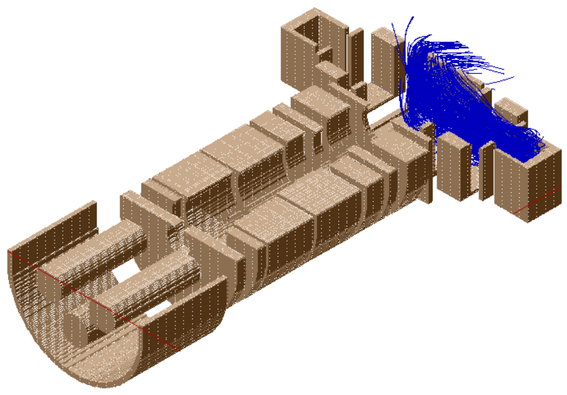


Fig. 4: Simulation: Trajectories of the electrons (only one filament).

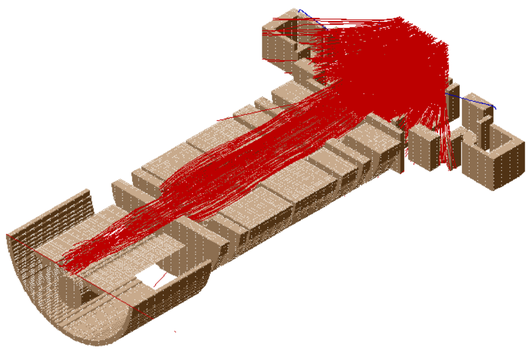


Fig. 5: Simulation: Trajectories of the cations with 121 m/z.

- Numerical simulations using SIMION[1] to assess the impact of voltages on the trajectories of electrons and ions.
- Simulated 70 eV electron trajectories (Fig.4) displays an efficient trajectory from the filament through the defocusing unit onto the sampling tip surface.
- The defocusing unit creates a large area electron beam, covering half of the surface.
- Ideally the entire sample is covered by electron bombardment.
- Lens system between filaments and sample lead to a desired electron beam.
- 67 % transmission for cations of 121 m/z (left, blue).
- The generated ions (Fig.5) are extracted from the sample by fitting potentials.
- 82 % of the generated ions reach the exit of the source, with the majority impinging on the last electrode (right, red).

Characterization and Performance

The prototype was assembled, and several issues were solved, including heat-sensitive materials and challenges in the electronics due to varying electrode voltages. The mass spectrum clearly shows EI signals, but separating them from sample-related signals remains a key challenge. Electron currents were monitored on several ion optical elements showing that a significant fraction of the emitted electrons were observed to reach the sample plate.

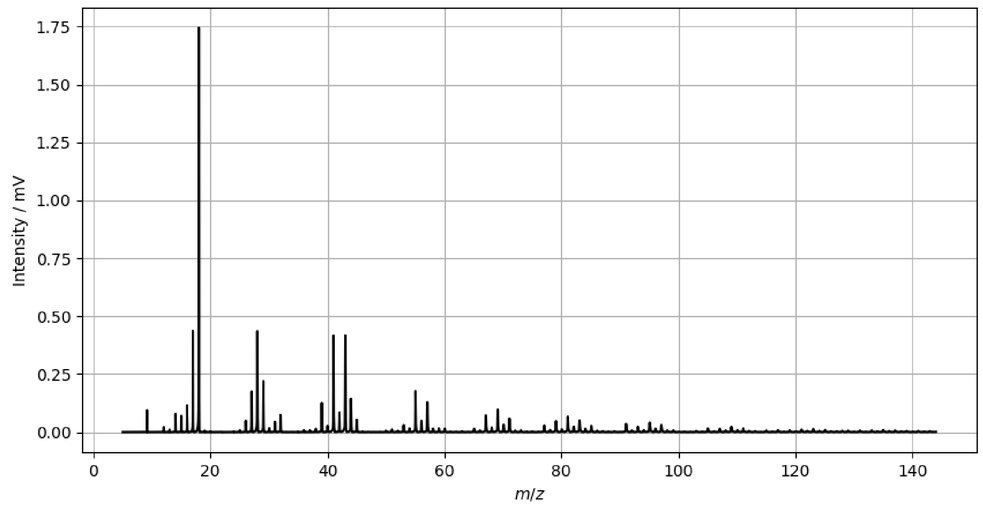


Fig. 6: Mass spectrum of the ion source after resolving technical issues.

Conclusion: Designed for analysis of trace gas from a plasma chamber with partial pressures below the LOD of the mass analyzer, this ion source enables indirect measurements where direct methods are not feasible. Simulations validated the concept and showed promising results. Despite minor troubleshooting, commissioning was successful. Ongoing efforts focus on characterization and further development.

References and COI Declaration

[1] D. A. Dahl. "Simion for the Personal Computer in Reflection"; doi: 10.1016/S1387-3806(00)00305-5 SIMION (v. 8. 1. 2. 30); ion optics and trajectory simulation program; http: simion.com
[2] cTOF time of flight mass spectrometer; *Tofwerk AG, Thun, Switzerland*

Financial support within the 14AMI project funded by the BMBF (16MEE0370) and the EU-CHIPS JU (101111948) is gratefully acknowledged.