Optimization of Direct Ionization of CO2 by Controlling the Gas Flow inside of a Beam-Target

G. A. Salazar Quintero, T. Ognibene

June 1, 2011

American Society for Mass Spectrometry Conference
Denver, CO, United States
June 5, 2011 through June 9, 2011
This document was prepared as an account of work sponsored by an agency of the United States government. Neither the United States government nor Lawrence Livermore National Security, LLC, nor any of their employees makes any warranty, expressed or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States government or Lawrence Livermore National Security, LLC. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States government or Lawrence Livermore National Security, LLC, and shall not be used for advertising or product endorsement purposes.
Fig. 1. The scheme of the CO2 injection system. A tank containing pressurized CO2 (Instrument grade 99.99% purity) sample loop was measured with 2 pressure analog-to-digital transducers connected at both ends. The CO2 flow the flow-meter dedicated for the He carrier gas coming from a pressurized He tank (Ultra high purity). The injection was connected to an electrically actuated GC injection valve with a 100 connected to a high-vacuum gas feedthrough (stainless steel tubing 30 cm long, 0.5 mm id, 1.6 mm od).

and converted it to grams of carbon based on ideal gas calculations. The pressures at both ends of the sample port, during the filling step, were kept within a relative difference of 4%. The software also was able to read and control was controlled with two micro control valves. A dedicated computer program continuously read the CO2 pressure system and the ion source were connected with a fused silica capillary (3 m long, 0.25 mm id, 0.35 mm od) and the ion source is only compatible with solid samples. The need of a direct ionization method to analyze gaseous samples in order to couple the AMS with other analytical instruments like gas chromatograph.

CONVENTIONALLY, Accelerator Mass Spectrometry needs to convert the biological samples into carbon graphite. The secondary ion source bombards the sample with Cs+ creating C- process that is only efficient with solid samples. In the ion source, CO2 is mixed with solid samples. This mix of a direct ionization method to directly analyze gaseous samples for CO2 is that the graphitization process is tedious and time consuming. Also there is a need of directly analyze gaseous samples due to the ion source is only compatible with solid samples. The need of a direct ionization method to analyze gaseous samples in order to couple the AMS with other analytical instruments like gas chromatograph.

We designed and optimized a target that directs a CO2 pulse onto a Ti surface where a Cs+ sputtering beam ionizes the CO2 to generate C-. These targets will be used for the direct ionization of CO2 pulses to enable the measurement of carbon isotope ratios in real time. The design was based on the results of ComsolTM simulations of the target configurations.

Computer simulations show that when the flow is directed, the gas pressure is higher at the Ti surface. Therefore, ionization efficiency should be higher for the directed-flow configuration.

Computer simulations showed that when the flow is directed, the gas pressure is higher at the Ti surface. Therefore, ionization efficiency should be higher for the directed-flow configuration. Computer simulations show that when the flow is directed, the gas pressure is higher at the Ti surface. Therefore, ionization efficiency should be higher for the directed-flow configuration.

Fig. 2  Possible fragmentations and negative ionization of CO2 during Cs+ beam bombardment. Fig. 3 Computer simulations of the insert configurations. a) Directed-flow showing the gas-pressure profile. The black arrows represent the direction of the velocity vectors; b) Same as (a) for the Diverging-flow. c) Pressure profile on the titanium surface (red line) for both configurations.

CONCLUSIONS

Direct ionization of CO2 was improved by computer-aided design and empirical optimization of a Cs+ beam target that directed the flow on a Ti surface where the beam is bombarding. By optimizing the parameters that affect the CO2 interaction with the Ti surface and Cs+ beam (amount of CO2, gas flow, Ti contact area and beam cross-section), effective ionization was obtained in the range of 1-2.5%. These results demonstrate the feasibility of using this ionization system for coupling HPLC with an online combustion interface with our AMS ion source.