C_{60} ToF-SIMS: A tool for high-resolution mapping of elements and organic compounds

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Experimental

A recent development in time-of-flight secondary ion mass spectrometry (ToF-SIMS) is the deployment of heavy cluster primary ion guns. Hereby desorption of secondary particles is less destructive and larger (organic) molecules can be detected intact, complementing the elemental information. Furthermore, the reduced penetration depth of the cluster ions causes less sputter damage like layer mixing and hence allows for shallower depth profiling.

We recently equipped one of our ToF-SIMS instruments [1, 2] with a 40 kV C_{60} primary ion gun from Ionoptika Ltd [3] for application in cosmochemistry. Measurements can be routinely performed with a lateral resolution of ~2 µm. Sub-micrometer resolution is possible although at the expense of intensity. Ultimately, this method enables the measurement of the 3D distribution of most major, minor and trace elements plus organic compounds on the (sub)micrometer scale. Our instrument is also equipped with a digital micro camera and a secondary electron detector to ease correlation with results from other techniques, e.g. electron microbeam methods. Additional non-resonant laser post ionization is almost operational. Its application will distinctively reduce detection limits and hence improve our capabilities to measure trace elements and isotopic compositions [2].

Application

Our first project is the examination of the aerogel capture medium used in the Stardust cometary sample return mission [4]. Surfaces of flight aerogel exposed to the cometary particle flux as well as unexposed will be analyzed. The aim of this study [5] is to investigate: (1) If direct deposition of organic compounds from the coma of comet Wild 2 can be identified on exposed aerogel surface. (2) If micrometer-sized impact structures are present, potentially accompanied by local enrichments of cometary matter including organic compounds. First results will be presented.

[1] Braun *et al.* (1998) *Rapid Commun. Mass Spectrom.* **12,** 1246–1252. [2] Henkel *et al.* (2007) *Rev. Sci. Instrum.* **78,** 055107. [3] Hill *et al.* (2006) *Appl. Surf. Sci.* **252,** 7304–7307. [4] Brownlee *et al.* (2006) *Science* **314,** 1711–1716. [5] Rost *et al.* (2008) *LPS* **XXXIX** #2110.

Characterization of simple fluids under confinement and at free interfaces using neutron scattering techniques

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The properties of simple and complex fluids confined in nano-porous earth and engineered materials can deviate significantly from bulk behaviour under the same thermodynamic conditions. Neutron scattering techniques can resolve the structure and mobility of imbibed fluids and of molecules in pores.

We used SANS to study the sorption properties of supercritical fluids inside mesoporous silica aerogel. The Adsorbed Phase Model [1] allows, for the first time, a means to quantify the physical properties of the adsorbed phase formed by fluids inside porous media in terms of the mean density and volume of the sorption phase. Knowledge of these quantities permits the model-free calculation of the absolute adsorption, a property relevant to application of the equation of adsorption and molecular modeling. The APM model has been applied to the SANS data obtained for sorption of carbon dioxide and sulphur hexafluoride in silica aerogel at supercritical conditions. Our results show clear evidence for fluid depletion for conditions above the critical density. The density and volume of the sorption phase change in a sensible, complex fashion as a function of pressure and temperature. As an extension to the SANS effort we recently explored the use of neutron reflectivity to assess the density profile of fluids near solid interfaces. Our initial study focused on the behavior of sulphur hexafluoride near a Si/SiO_2 interface to confirm the existence of a fluid depletion zone near the surface at fluid densities near and above the critical density. Ultimately, the combination of SANS and neutron reflectivity data and molecular dynamics modeling will provide a more fundamentally-rigorous understanding of the interplay between surface and confinement effects.

[1] G. Rother *et al*. (2007) *J. Phys. Chem. C* **111**, 15736.