Background

Secondary Ion Mass Spectrometry (SIMS) has developed over the years into a powerful analytical tool for elemental analysis, particularly in materials such as semiconductors. Recently these techniques have been utilized to make molecular concentration images (maps) of surfaces. Secondary Ion Mass Spectrometry (SIMS) has progressed a long way to produce high resolution molecular concentration images of surfaces with lateral resolution below a micron. State-of-the-art SIMS equipment employs cluster beams to enhance the yield of large molecular ions and is capable of mapping the presence of molecular material with masses up to several tens of kDa. New developments are pushing forward with depth profiling of molecular materials to provide ultimately a complete 3D image of the analyzed material. The only drawback to this technique is that it uses keV ions and clusters to sputter intact molecular species into the gas phase for analysis. These keV ions cannot penetrate more than a few microns in ambient conditions and so the analysis must be performed in vacuum.

Atmospheric Pressure Mass Spectrometric techniques currently available include Matrix Assisted Laser Desorption Ionisation spectroscopy (MALDI), Direct Analysis in Real Time (DART) and Desorption Electro Spray Ionisation spectroscopy (DESI), which are limited by the resolution of the probe beam to about 30 microns at best in the case of MALDI and millimetres in the case of DART and DESI with no real potential for mapping. Also the choice of the matrix (in MALDI) or analyte (in DESI) can influence the detection limits of some molecular species. Consequently care has to be taken when analysing samples of unknown molecular composition. Laser Ablation Inductively Coupled Plasma Mass Spectrometry (LA-ICP-MS) can be performed at relatively high spatial resolution (~10 microns) but the technique destroys all molecular information in the laser ablation and ionization phases. To date there is not a mass spectroscopy technique capable of providing high mass molecular maps in ambient pressure conditions with high spatial resolution.

In the 1970s a fission fragment technique known as Plasma Desorption Mass Spectrometry (PDMS) was developed which utilized the high electronic energy deposition caused by the slowing down of a fission fragment from a californium source. The high energy density generated close to the surface of a biological sample was found to cause sputtering of intact large molecules from organic samples. The initial promise demonstrated by this technique was soon overtaken by the invention of MALDI.

It is possible to extract MeV ions out of the vacuum system and into air through a thin window. This technique has been used extensively in the past with protons and helium ions to perform elemental analysis of objects in ambient conditions using conventional Ion Beam Analysis (IBA MeV) techniques, ranging from Particle Induced X-ray Emission (PIXE) and Particle Induced Gamma-ray Emission (PIGE) to Rutherford Backscattering Spectroscopy (RBS), Ion Beam Induced Charge (IBIC) and Ion Beam Induced Luminescence (IBIL). It has also been demonstrated that it is possible to use MeV heavy ion beams to produce secondary ions from a molecular solid surface in a PDMS mode (or MeV-SIMS). A conventional scanning microprobe using a heavy ion such as O^{4+} or Cl^{4+} can be used to produce MeV-SIMS maps of molecular material. It has also been able to demonstrate that simultaneous
PIXE, RBS and SIMS measurements can be made using the same ion beam providing complimentary measurements of the sample.

**Applications**

A number of key areas would benefit from a high resolution ambient pressure molecular imaging system. These include: Archaeometry, Geological & Environmental Sciences, Forensics and Biomedical Sciences.

**Aims**

To bring together MeV-SIMS practitioners and experts from related techniques, and personnel from other accelerator facilities who might be considering entering this technological area.

Encourage setting up of inter-comparisons of sample imaging with other competitive and complimentary techniques. These would provide a useful insight into the strengths and weaknesses of this emerging technology.

**Objectives of the Technical Meeting**

a) Identify and address weaknesses in the understanding of the fundamentals of molecule desorption from surfaces by fast heavy ions  
b) Move towards an understanding of ionization of the desorbed molecules  
c) Compare instrumentation technologies  
d) Address issues of sample preparation and data interpretation  
e) Outline needs for molecular imaging, in particular under ambient conditions, in such fields as medicine, forensics and cultural heritage issues  
f) Bring into the field new practitioners from accelerator laboratories, particularly from developing countries