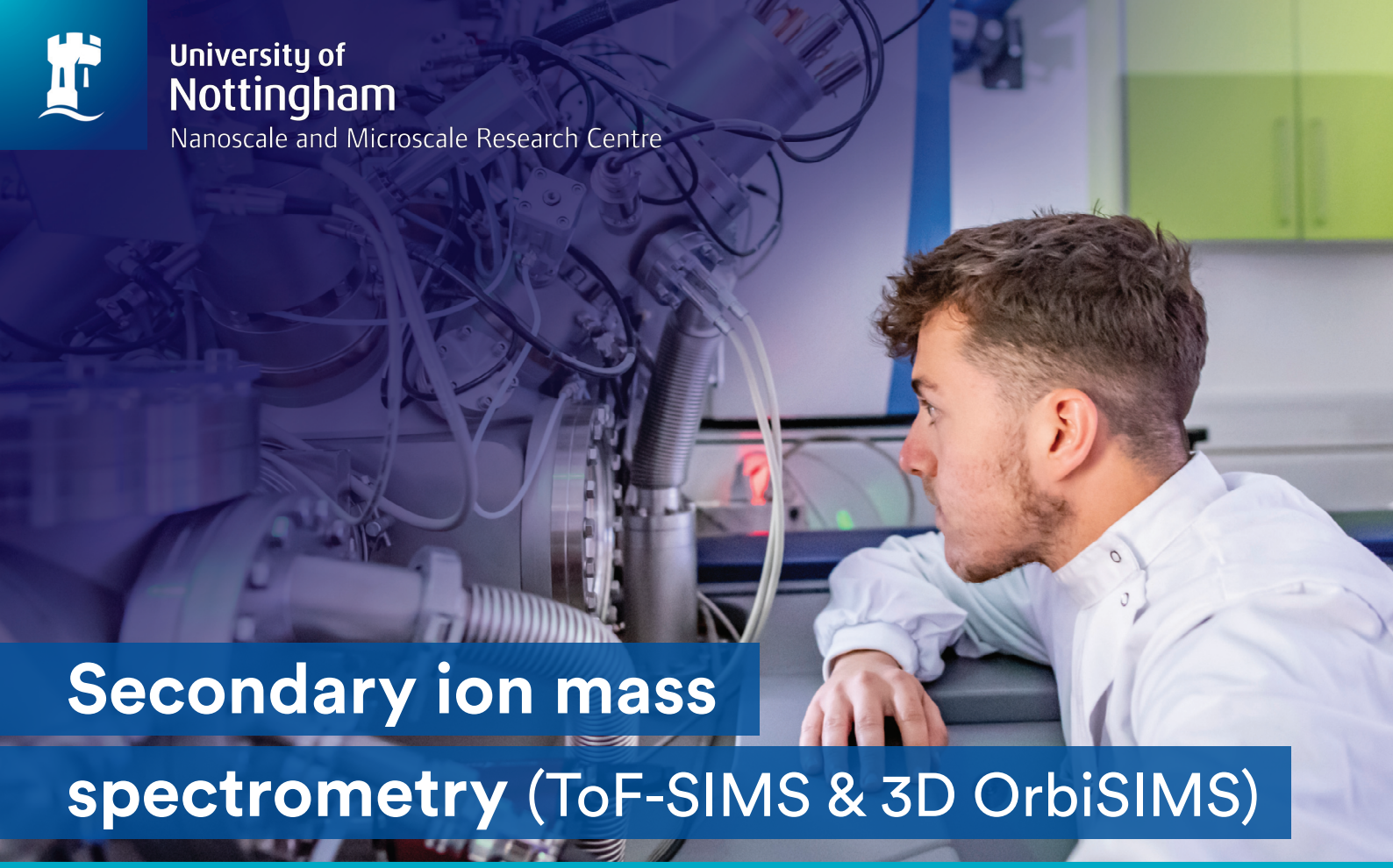
University of Nottingham
Nanoscale and Microscale Research Centre



Secondary ion mass spectrometry (ToF-SIMS & 3D OrbiSIMS)

Secondary ion mass spectrometry is used to characterise the surface chemistry of a material. A beam of primary ions impacts the surface and liberates secondary ions from the sample which are then analysed in turn to produce mass spectra. The lateral distribution of chemical species (mapping) or their intensity with depth (depth profiling) can then be carried out.

The combination of a time-of-flight secondary ion mass spectrometer (ToF-SIMS) with hybrid OrbiTrap™ functionality provides an array of analytical options to provide 3D chemical analysis with exceptional surface sensitivity (1-3 nm), high mass and spatial resolutions.

Capabilities

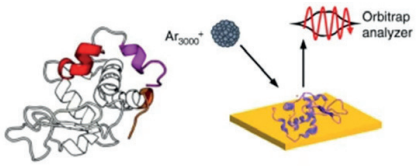
- Label-free large molecule identification (> m/z 1000)
- Sensitive trace element identification (ppm)
- Chemical mapping (down to a nm scale)
- Depth profiling of inorganics and organics

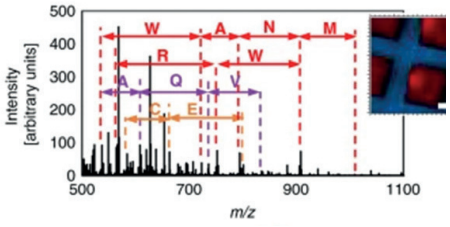
Typical applications

- Identification of unknown organic species in solids
- Contaminant identification and distribution
- Surface (such as coatings, films, deposits) composition and integrity
- 3D permeation assessment of active pharmaceutical ingredients
- Spatial resolution of chemical components.
- High throughput screening of polymers

In-situ protein identification for next generation biomaterials and tissue analysis

Using the ballistic fragmentation and high accuracy of the 3D OrbiSIMS, 16 undigested proteins were identified in-situ (in their native state). This was achieved without a chemical label, enzymatic digestion or use of a specific matrix. Using the ballistic approach the concentration of key proteins was tracked into human skin. The ability to directly measure proteins in their native state using a surface analysis technique has significant potential application in furthering the understanding of diseases and the development of new bio-materials.

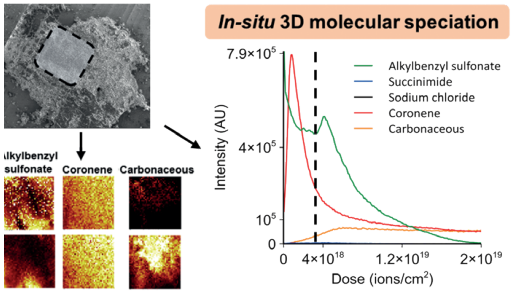




AM Kotowska, GF Trindade, PM Mendes et al. Protein identification by 3D OrbiSIMS to facilitate in situ imaging and depth profiling. *Nature Communications* 11 (2020), 5832. doi.org/10.1038/s41467-020-19445-x

3D insight into the molecular composition and formation of polluting engine deposits

Formation of deposits in internal combustion engines causes increased emissions and lower engine efficiency. Using the 3D OrbiSIMS technique it was possible to depth profile and image these complex layered materials and, coupled with sophisticated chemical filtering using molecular formula prediction for data processing, a comprehensive molecular characterisation of petroleum deposits was performed. Argon gas cluster depth profiles tracked the fate of molecules once deposited on the engine surface and unveiled plausible formation pathways of deposits for the first time. The combined insight into the composition, origin and formation of deposits will help mitigate the use of solubilising fuel additives and help reduce worldwide vehicle emissions.

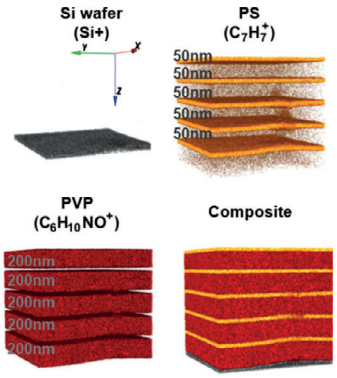


M Edney, J Lamb, M Spanu, E Smith, E Steer, E Wilmot, J Reid, J Barker, M Alexander, C Snape and D Scurr. ACS *Applied Materials and Interfaces* 12 (2020), 51026–51035.

MK Edney, AM Kotowska, M Spanu, GF Trindade, E Wilmot, J Reid, J Barker, JW Aylott, AG Shard, MR Alexander, CE Snape, DJ Scurr. *Analytical Chemistry* 94 (2022), 4703–4711.

3D ToF-SIMS imaging of polymer multi-layer films

ToF-SIMS imaging with argon cluster sputter depth profiling can provide a detailed insight into the three-dimensional chemical composition of organic material structures. 3D chemical images can provide information regarding the structure of multi-layer systems which can be used to inform future manufacturing and development. Outputs include sample layer chemistry, homogeneity, thickness and interface widths. Here we can see the analysis of spin-cast multi-layers comprising alternating polystyrene (PS) and polyvinylpyrrolidone (PVP) layers. The quality of the data allows a detailed analysis of the chemical structure of these systems, revealing minor imperfections within the polymer layers.



J Bailey, R Havelund, JS Sharp, AG Shard, I Gilmore, MR Alexander, DJ Scurr. ACS *Applied Matererials and Interfaces* 7 (2015), 2654–2659.

Our facilities

ION-TOF (GmBH) ToF SIMS V

- Liquid metal (Bin+n) ion gun (LMIG) for spectroscopy and imaging at a spatial resolution of ~ 200 nm.
- Argon gas cluster source for high-resolution depth. profiling of organic materials (polymers and biological samples) and 3D chemical characterisation.
- Mass sensitivity down to ppm (femtomole).
- A 5-axis multi-sample stage is fully automated and provides rotation for high-resolution (nm) depth profiling (Cs+ or Ar GCIB sources).
- Reflectron ToF mass analyser gives mass resolution > 13000 at m/z = 29.
- Chemical imaging of surface areas from the µm to cm scale.
- 3D elemental mapping possible.
- Sample size accommodation from a few mm up to ~ 10 cm.

Ion-TOF (GmbH) HybridSIMS

- ToF or OrbitrapTM analysis of organic and inorganic samples including petroleum deposits, biological materials (protein identification, skin, hair, leaves and others), polymers, semi-conductors, insulators, powders, foils and microarrays.
- High mass resolution spectrometry (>240,000 and 11,000 amu for the OrbiTrap and the ToF, respectively).
- High spatial resolution chemical imaging (<70 nm).
- Mass sensitivity down to ppm (femtomole).
- Gas cluster ion beam sputtering for controlled depth profile analysis of organics.
- Biosafety Level 2 (BSL2) preparation and analysis environment for cell/tissue analysis including cryogenic sample preparation facility, including high pressure freezing, freeze drying, cryo-ultramicrotomy and more.
- Chemical filtering and multivariate analysis software and expertise for complex chemometric data analysis.

Find out how ToF/3D OrbiSIMS could help with your applications, designs or solutions:

nmrcenquiries@nottingham.ac.uk | +44 (0)115 951 5046

nottingham.ac.uk/nmrc