PROJECT TITLE: TOF SIMS—Bridging materials science and palaeontology

DTP Research Theme(s): Dynamic Earth, Living World

Lead Institution: University of Bristol

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Project keywords: palaeobiology, taphonomy, materials science, mass spectroscopy

The J105 SIMS.  https://www.ionoptika.com

Example of how it is possible to map secondary molecular ions across a surface with marked relief using the J105 SIMS. This is a frog embryo and different lipids are characterised across a spherical surface. From Tian et al. 2014 http://www.jlr.org/content/55/9/1970.full

Project Background
The fossil record holds crucial evidence for the nature and evolution of the biosphere. Exceptionally preserved fossils hold crucial cues to the nature of extinct organisms, but due to their rarity they are precious and difficult to probe. There are still major conceptual gaps in our understanding of fossilisation processes: What processes lead to preservation and what original biomolecules are retained and how are they altered during diagenesis?

Together with IONOPTIKA this PhD project will allow the candidate to develop a new and promising analytical instrument for fossils analysis. Their new and ground breaking J105 can not only analyse rough surfaces with perfect mass resolution, but with novel primary ion sources, more molecular data is obtained with much better collection of higher mass secondary organic ions. TOF SIMS allow researchers to collect mass spectroscopic data in a minimally destructive fashion and furthermore being able to spatially map the composition across a surface. This means that fossils that may preserve several organic molecules and tissues can be probed.

Project Aims and Methods
The project includes 3 main components

1. **Optimising the J105 for analysing smaller and larger rock samples**
   Due to the nature of fossil samples that need to be evacuated and the potential of these to charge under the high current, it is necessary to develop the experimental protocol and understand the best practice for sample preparation and machine configuration for different samples

2. **Develop standard spectra from extant and experimentally fossilised organic compounds.**
   The use of different primary ion sources changes the spectral composition of molecular fragments that the machine collect. In order to compare spectra and diagnose compounds, it is necessary to collect data from extant samples as well as artificially matured samples (cooked under high pressure and temperature) in order to develop a reference library.

3. **Demonstrate the utility of J105 in fossil analysis, developing integrative research projects and answer scientific questions (taphonomic, ecological, evolutionary).**
   The last component provide the student to develop their own research project (s) and with the knowledge from 1. and 2. to answer novel and important palaeobiological questions.
Methods

**Mass spectroscopy.** The mass spectroscopic data will be collected on the J105 TOF SIMS. Other mass spectroscopic facilities can be implemented for comparative and validatory purposes. TOF SIMS data provide secondary ion spectra from individual data points across a larger area. These can be investigated by mapping individual secondary ions across a specimen. Secondary ions need to be identified and spectral shape can be compared visually and using statistical methods. **Experimental taphonomy.** Organic materials undergo transformations during geological burial which ultimately may transform the compound into volatiles, or into graphite. Experimental methods can elucidate these processes. **Chemical extraction and purification of molecules.** Several compounds are not available commercially. A great part of this project therefore entails purifying organic molecules using organic chemistry and molecular biological procedures.

Candidate Requirements

The candidate can have either a chemistry, materials science or geology/biology background. The key aspect for a successful candidate will be to be willing to develop and expand their repertoire of transferrable skills.

**CASE Partner**

IONOPTIKA developed the J105 TOF SIMS, which is the most innovative TOF SIMS developed in the last 20 years. Its potential in materials science, medicine as well as in palaeontology are still largely untapped. Therefore, the unique opportunity to work closely with IONOPTIKA sets this project apart as a unique opportunity for the candidate to obtain exclusive expertise and research.

Training

The student will get training in mass spectroscopic analysis, operating a TOF SIMS, experimental taphonomy, electron microscopy as well as several disciplines within palaeobiology. This project not only equip a student for different directions within the private sector, but is also a possibility for becoming an integrative researcher and teacher within academia.

Background reading list


Links:

School URL – [http://www.bristol.ac.uk/earthsciences/courses/postgraduate/](http://www.bristol.ac.uk/earthsciences/courses/postgraduate/)

NERC GW4+ DTP Website: [http://nercgw4plus.ac.uk/](http://nercgw4plus.ac.uk/)

Bristol NERC GW4+ DTP Prospectus: [http://www.bristol.ac.uk/study/postgraduate/2019/doctoral/phd-great-western-four-dtp/](http://www.bristol.ac.uk/study/postgraduate/2019/doctoral/phd-great-western-four-dtp/)

Application deadline: 16:00 GMT, Monday 7 January 2019

How to apply to the University of Bristol: [http://www.bristol.ac.uk/study/postgraduate/apply/](http://www.bristol.ac.uk/study/postgraduate/apply/)

General Enquiries: Bristol NERC GW4+ DTP Administrator Email: [bristol-nercgw4plusdtp-admin@bristol.ac.uk](mailto:bristol-nercgw4plusdtp-admin@bristol.ac.uk)