

# Sunday Afternoon, September 18, 2022

## SIMS School: IUVSTA Short Courses

### Room Great Lakes A2-A3 - Session SC-SuP

#### SIMS School - IUVSTA Short Courses

11:30am **SC-SuP-1 Fundamentals of SIMS - Views from Ground Zero and Beyond**, *Arnaud Delcorte*, Université Catholique de Louvain, Belgium

**INVITED**

An initial particle impact event – “big bang” in the universe of the SIMS aficionados – induces the generation of free and stable ions from solid samples, the signature of which eventually forms a *secondary ion mass spectrum*. The once hypothetical representations and/or qualitative models of this founding event have given way to more quantitative predictions in the last two decades (even for complex samples, e.g. the sputtering yields of argon clusters in organics), owing largely to the progress of molecular dynamics computer simulations. In this short course, the basics of kiloelectronvolt cluster impacts in atomic and molecular solids are reviewed using the magnifying lens of the microscopic models. For instance, (large) cluster and molecular impacts differ radically from single atom impacts in that they systematically induce collective motions in the solid (pressure waves, correlated atomic and molecular motions, crater formation as opposed to “linear cascades”), which make their action resemble (tiny) meteorite collisions. The mechanisms of projectile penetration, energy deposition, atomic motion and damage in the solid, determined in the first few picoseconds of the impact event are described. Beyond the “ground zero” of the cluster impact, the emission of atoms, fragments and molecules are discussed, with an emphasis on the conditions of intact molecular emission and their links to the molecule internal energy uptake and the projectile properties. Finally, the questions of ionization and matrix effects – annoying but central to SIMS – are considered and unresolved fundamental issues are delineated.

12:30pm **SC-SuP-7 SIMS Analysis of Biological Materials**, *Michael J. Taylor*, Pacific Northwest National Laboratory

**INVITED**

1:30pm **SC-SuP-13 SIMS Inorganic Depth Profiling**, *Jerry Hunter*, University of Wisconsin

**INVITED**

3:00pm **SC-SuP-22 Multivariate Analysis Methods for Secondary Ion Mass Spectrometry and Related Techniques**, *Jean-Paul Barnes*, CEA-Leti, France

**INVITED**

The complexity of secondary ion mass spectrometry data can make interpretation difficult and time consuming in many cases. In order to make sense of data sets, many researchers choose to apply multivariate analysis (MVA) methods or more recently machine learning approaches. This short course will give an overview, and the basic principles of the most commonly used multivariate and machine learning methods used for SIMS data, but also for other similar analytical techniques or techniques that are often correlated with SIMS data.

Using such methods may on the one hand seem daunting at first, or on the other hand tempting as a quick-fix to interpret a data set. This course will attempt to demystify the available methods and how to tackle the data acquisition and pre-processing steps in order to obtain reliable multivariate analysis results. We will address practical examples of how to plan a SIMS experiment for multivariate analysis and what can go wrong when trying to use multivariate analysis on data sets that were not initially designed for this purpose.

For example, among the multivariate analysis methods, principal component analysis (PCA) is one of the most employed approaches. This method allows the orthogonal directions (combination of mass channels) of maximum variance in a dataset to be found. This can then be used to identify the chemistry present in a data set and identify areas of different composition in an image, depth profile or group together spectra from different samples that have similar chemistry. Practical examples will be given of how multivariate analysis can be used to solve problems in both a research and an industrial context. In terms of perspectives, the potential of new and emerging algorithms to be applied to SIMS data will be discussed.

4:00pm **SC-SuP-28 SIMS Analysis of Organic Materials with Industrial Applications**, *Michaëleen Pacholski*, Dow Chemical Company

**INVITED**

SIMS analysis is a valuable tool in a large analytical group. In this presentation examples from an industrial lab will be shown highlighting how SIMS fits in to solving the analytical puzzles presented. These will

include projects using multiple analytical techniques, projects focusing on adhesion (or lack thereof), combining XPS and SIMS data to understand concentrations, multilayer sample analysis, etc. Since GCIB (gas cluster ion beam) sources are now widely available, SIMS not only aids in surface analysis, but also contributes to our understanding of interfaces through depth profiling. Additionally, tips for setting yourself up for success, from sample preparation to reporting results will be shared.

## Author Index

**Bold page numbers indicate presenter**

— B —

Barnes, J.: SC-SuP-22, **1**

— D —

Delcorte, A.: SC-SuP-1, **1**

— H —

Hunter, J.: SC-SuP-13, **1**

— P —

Pacholski, M.: SC-SuP-28, **1**

— T —

Taylor, M.: SC-SuP-7, **1**