Information from Complexity: Challenges of TOF-SIMS Data Interpretation

Prof David Castner, University of Washington
Co-authors:
Daniel J. Graham, University of Washington

TOF-SIMS data is complex. This is true even of the simplest systems. Yet it is within this complexity that information about sample composition, molecular orientation, surface order, chemical bonding, sample purity, etc. is contained. The challenge is how to easily extract this information from the spectra. Fortunately multivariate analysis (MVA) has shown promise in taming the complexity challenges presented by TOF-SIMS spectra. TOF-SIMS data is well suited for this type of analytical methodology since the spectra generated are inherently multivariate. Multiple peaks are generated from the same surface molecules, and their relative yields are often interrelated. MVA methods allow utilization of the entire spectrum to determine which peaks correlate with various surface treatments or chemistry changes. The success of MVA methods such as principal components analysis (PCA) and partial least squares (PLS) has lead to a great increase in the interest of MVA in TOF-SIMS data processing. Nevertheless, we have only begun exploring the capabilities of what methods such as PCA and PLS can do, and possibly more importantly, no standards have been established for data preprocessing before these methods are applied. To realize the full power of these methods we will need to understand better what data to use to answer a given question, how to optimally process the data before applying MVA and how to correctly interpret the outcomes from the analysis. Even with these caveats to MVA, PCA and PLS have shown great success in the analysis of self-assembled monolayers, proteins, polymers, and extra cellular matrix materials. PCA has also enabled accelerated analysis and interpretation of TOF-SIMS imaging data sets that present an even more complexity due to their large size and low signal to noise ratios.

Though much has been done to improve the methodologies of TOF-SIMS data processing and analysis, there are still many challenges that stand between the complexities of the TOF-SIMS fragmentation pattern and the information contained therein. To meet these challenges MVA methods have been explored. For example, our group has explored how using model systems in conjunction with PCA can extract information about the TOF-SIMS fragmentation process. PCA has been applied to the identification of proteins based solely on the fragmentation pattern of the amino acids. PLS has been applied to the quantification of binary and ternary protein mixtures. Image processing methods and PCA are being explored to improve spatial resolution and species identification in TOF-SIMS imaging.

The challenges of TOF-SIMS data interpretation will only get more complex. This is already being demonstrated with the analysis of cells, tissues and the increasingly complex engineered surfaces used in research and development today. These developments will increase the need for well-controlled MVA methodologies. Standards need to be established in the proper application of MVA methods to TOF-SIMS data. Model systems need to be studied to generate databases of peaks related to the various surface components of cells and tissues. The fragmentation process of the various ion beams used today need to be more fully understood. Moving forward in these areas will aide in unlocking the information encoded in the complexities of TOF-SIMS spectra.