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Tutorial SC5

Practical TOF-SIMS

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The Time-of-Flight Secondary Ion Mass Spectrometry (TOF-SIMS) technique was found to have practical uses almost from its inception, so much so that research into its application has far out-sped research that explored how it works.¹ Despite the fact that TOF-SIMS results are far from chaotic (small differences in sample surfaces do not produce large differences in TOF-SIMS measurements), analysts must take care in planning their analyses, and in interpreting their data.² This tutorial will provide an outline of how to use TOF-SIMS for surface analysis in such a way as to use it to greatest advantage, how to interpret the data, and how to avoid common pitfalls in data interpretation.

I will outline ways to interpret the mass spectra when it is necessary to identify unknowns. SIMS mass spectra differ from EI mass spectra but also have some similarities.³ Clues in SIMS spectra include exact mass positions, odd and even nominal masses of ions, series of peaks with identical mass differences, as well as isotope and other patterns. Unlike most other mass spectrometry methods, SIMS suffers from the absence of a chromatography method that can separate compounds prior to ion formation, making it likely that the spectrum derives from a mixture of species. With the increasing adoption of MS/MS techniques in TOF-SIMS the identification of unknowns becomes less problematic, but there is still the need to select precursors, and MS/MS is far from available in every laboratory.

I shall touch on the fundamentals as we understand them behind ion formation and, as important, ion survival, and thus how the famous SIMS matrix effects arise. In particular, the varied ability for electrons to tunnel from the surface to an ion leaving the surface can change signal intensities by orders of magnitude. Keeping these fundamentals in mind, analysts can judge how to interpret their results, and when differences in surfaces are less or more likely to be problematic. The tutorial will also cover what steps need to be taken in order to use TOF-SIMS quantitatively.

¹ A. Benninghoven, H.W. Werner, and F.G. Rudenauer, *Secondary Ion Mass Spectrometry: Basic Concepts, Instrumental Aspects, Applications.* (Wiley Interscience, 1986).

² A.M. Spool, *The Practice of Tof-Sims: Time of Flight Secondary Ion Mass Spectrometry* (Momentum Press, 2016).

³ A.M. Spool, "Interpretation of static secondary ion spectra," SURFACE AND INTERFACE ANALYSIS **36**(3), 264–274 (2004).