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TOF-SIMS: Instrument innovations and industrial applications

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In the early 1980s, TOF-SIMS has been developed to provide detailed elemental and molecular information from surfaces under static conditions. Over the years, continuous development has transformed TOF-SIMS from a pure surface spectrometry tool into an extreme flexible and versatile technique providing not only high mass resolution spectrometry, but also imaging performance in the sub 100 nm range as well as depth profiling of inorganic and organic materials with high sensitivity and reproducibility.

One key to success has been the introduction of new ion sources. By using field emission sources, the imaging performance could be significantly improved. Best achieved lateral resolution is in the 20 nm range and therefore close to the dimension of the sputter cascade, the physical limit. Another important step was the application of cluster ion sources for sputtering of organic materials. In particular the introduction of the gas cluster ion beams (GCIB) made organic depth profiling feasible.

While new ion sources have expanded the scope of TOF-SIMS instruments significantly, TOF-SIMS analyzers lacked the mass resolution and mass accuracy. Although state-of-the-art TOF-SIMS instruments are reaching a mass resolution ($m/\Delta m$) of 30.000 and a mass accuracy in the range of a few ppm, it is not sufficient to unambiguously identify a mass peak due to the enormous number of organic molecules in the mass range of interest. Adding MS/MS capabilities can further increase confidence in the peak assignment and as the MS/MS fragment ion spectrum is almost independent from the ion generation of the precursor, one can benefit from the large number of reference spectra collected in various libraries.

While the discussed performance represents the limit attainable with recent TOF-SIMS instrumentation, further improvement is achieved by combining an OrbitrapTM-based mass analyzer (QExactiveTM HF, Thermo Fisher ScientificTM) with a high-end TOF-SIMS system (Hybrid SIMS). The instrument provides highest mass resolution (> 240,000) and highest mass accuracy (< 1ppm) and MS/MS capability at full mass resolution.

In this contribution an overview of recent advances in TOF-SIMS instrumentation and data evaluation will be presented which extend existing applications or even make new applications possible. Among the improvements discussed will be key instrumental values of the TOF-SIMS mass spectrometer such as mass resolution and lateral resolution, as well as improvements that are based on the integration of additional analytical components or due to the combination with complementary techniques.