Exploring the Frontiers of SIMS: Pushing Forward Together

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The continuous evolution of Secondary Ion Mass Spectrometry (SIMS) has been driven by the synergy of innovative instrumentation and expanding application fields. Gas Cluster Ion Beams(GCIBs), originally developed for advanced material processing, have now become indispensable tools in cutting-edge semiconductor manufacturing. Thanks to the invaluable contributions of numerous collaborators, extending the application of GCIBs to surface analysis has brought about an unprecedented paradigm shift, opening up entirely new dimensions in molecular imaging and depth profiling.

Accurate molecular identification has long been a major challenge in SIMS, but recent innovations such as Orbitrap and MS/MS analyzers have dramatically improved this capability. However, the ultimate sensitivity remains strictly constrained by the secondary ion yield. Since a significant majority of sputtered species leave the surface as neutral particles, understanding their molecular structures is crucial for defining the theoretical limits of SIMS. Prior to the advent of GCIBs, it was believed that most sputtered organic molecules were fragmented during ion-collisions. In recent investigations, we successfully characterized the molecular structure of these neutral species using advanced capturing techniques.[1] Remarkably, a substantial fraction of the sputtered neutral particles actually remain entirely intact during the cluster ion bombardment. Quantitative measurements using polymer systems revealed that the survival rate—the ratio of unfragmented neutral molecules to total sputtered species—reaches several percent, though it gradually scales down with increasing molecular weight.

These findings unveil a profound opportunity: if these abundant, intact neutral particles can be efficiently post-ionized, the secondary ion yield could be boosted by several orders of magnitude. Although implementing an optimal post-ionization framework within advanced mass spectrometers is a highly challenging subject, drawing inspiration from related disciplines like MALDI-2 suggests that breakthroughs are within reach. Pushing the frontiers of SIMS requires collective exploration into novel ionization methodologies, paving the way toward ultimate sensitivity together.

[1] “Molecular weight dependence of molecular damage to polyethylene glycol (PEG) molecules by sputtering with Ar gas cluster ion beam”, Y. Mizutani, M. Fujii, T. Seki and J. Matsuo, J. Vac. Sci. Technol. B 43, 044007 (2025): https://doi.org/10.1116/6.0004662