Latest applications of ToF-SIMS characterization for next-generation electronic materials

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Developing new materials other than silicon for next-generation electronic devices is one of the most crucial topics for emerging technologies. However, the complexity of these materials in their structures makes them particularly challenging for numerous characterization and analytical techniques for exploring the chemical composition and the potential chemical reactions such as degradation, diffusion, or doping. Among the most suitable characterization tool, time-of-flight secondary ion mass spectrometry (ToF-SIMS) is a very sensitive surface analytical technique providing detailed elemental and molecular information about the surface, thin layers, interfaces, and full three-dimensional analysis of the samples, as shown in figure 1. Recently, advances in instrumentation and sample preparation have permitted a rapid development for characterizing a wide range of applications such as next-generation electronic materials.

Thanks to the advances in ToF-SIMS characterization, understanding the chemical composition and the different components in the complex structures is now possible. This instrument progress permits a deeper exploration and a better knowledge of next-generation electronic materials such as batteries, perovskites, and 2D materials. This work will present different approaches to preparing and investigating various materials and devices.

After a brief introduction of ToF-SIMS and a short overview of the analytical challenges, we will present a few studies on advanced materials and devices.

Firstly, we will focus on the characterization of batteries. Initially, we will discuss the sample preparation and our specific setup for transferring the specimens from the inert atmosphere in the glovebox to the ultra-high vacuum chamber of our instrument. Then, we will illustrate the possibility to study the reversibility of the chemical composition between pristine, charged, and discharged batteries using surface mass spectrometry by ToF-SIMS [1] and next, we will compare three methods of cross-sectioning used to identify the interfacial species in a composite cathode [2].

Later, we will discuss the analysis of perovskites by ToF-SIMS. This type of materials is particularly interesting on a few levels as they are often hybrid, i.e. that the material can combine an organic-inorganic halide perovskite and that the film can also be integrated into a complex multilayer device such as a photovoltaic solar cell. Thus, we will show a study of an in-depth distribution of the 3D/2D heterostructures for perovskite solar cells where we have been able to identify individually the 3D and 2D heterostructures along with the depth of the film. Then, we will illustrate the characterization of interdiffusion in quasi-2D perovskite light-emitting diodes as a function of the organic ligand layer inserted into the perovskite crystals.

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Finally, we will finish by demonstrating how the retrospective analysis using ToF-SIMS can be very powerful and useful for exploring any single feature in 2D materials [3, 4]. Typically, ToF-SIMS acquisition is recording a full mass range spectrum per pixel (or voxel), which permits to isolate and to decorrelate specific regions of interest for resolving interfaces, diffusion, and doping in thin 2D structures. In particular, we will present how to treat a 3D volume image of a multilayer perovskite device for extracting useful information.
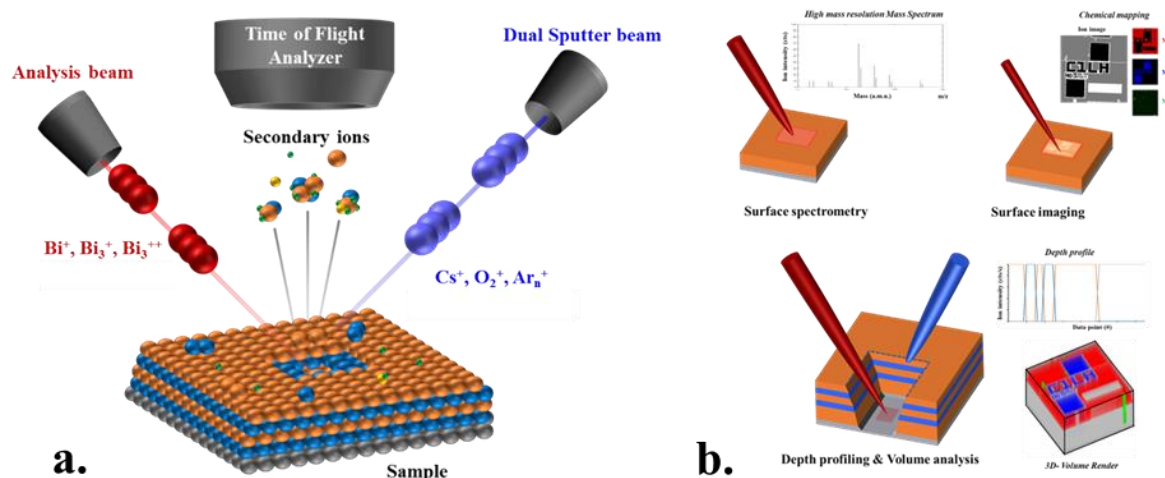

Figure 1. Schematic for analysis of a surface by time-of-flight secondary ion mass spectrometry (ToF-SIMS) showing (left) the sputtering process that generates secondary ions, and (right) modes of analysis that include acquisition of a surface mass spectrum, a mass-spectrometry (MS) image, and a depth profile of the material which produces a 3-D volume rendered dataset. Each pixel contains a full-range mass spectrum for that region of the sample.

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