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Full Length Article

# Methodological development of topographic correction in 2D/3D ToF-SIMS images using AFM images



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## ABSTRACT

Time-of-flight secondary-ion mass spectrometry (ToF-SIMS) is an emerging technique that provides chemical information directly from the surface of electronic materials, e.g. OLED and solar cell. It is very versatile and highly sensitive mass spectrometric technique that provides surface molecular information with their lateral distribution as a two-dimensional (2D) molecular image. Extending the usefulness of ToF-SIMS, a 3D molecular image can be generated by acquiring multiple 2D images in a stack. These imaging techniques by ToF-SIMS provide an insight into understanding the complex structures of unknown composition in electronic material. However, one drawback in ToF-SIMS is not able to represent topographical information in 2D and 3D mapping images. To overcome this technical limitation, topographic information by ex-situ technique such as atomic force microscopy (AFM) has been combined with chemical information from SIMS that provides both chemical and physical information in one image. The key to combine two different images obtained from ToF-SIMS and AFM techniques is to develop the image processing algorithm, which performs resize and alignment by comparing the specific pixel information of each image. In this work, we present methodological development of the semiautomatic alignment and the 3D structure interpolation system for the combination of 2D/3D images obtained by ToF-SIMS and AFM measurements, which allows providing useful analytical information in a single representation.

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## 1. Introduction

Secondary ion mass spectrometry (SIMS) is a highly refined mass spectrometry (MS) technique specialized for surface analysis by detection of ionized particles (i.e., secondary ions) on the surface of the sample [1]. Imaging mass spectrometry by SIMS is a powerful technique combining the chemical specificity and parallel detection of mass spectrometry with microscopic imaging capabilities [2]. The ability to simultaneously obtain chemical images from all analytes on the sample surface provides spatial distribution of interesting species from atomic to macromolecules and their chemical organization. However, one drawback in SIMS imaging cannot provide topographical information on the surface because the secondary ions sputtered from the topmost surface are detected in a planar way while the surface topography is neglected [3].

The lack of the topography in 2-dimensional (2D) SIMS images can cause the surface topography-induced artifacts such as the edge-darkening artifact at the lower lying surface next to the accentuated surface structures [3]. Moreover 3-dimensional (3D)

SIMS images have more chance to represent the laterally distorted element distributions, because the data acquisition is combined with the surface erosion by the sputtering process. The application of SIMS analysis in electronic devices are more and more increasing since they have been developed into more complex and smaller structures [4,5]. For example, organic light emitting diodes (OLED) device has very complex structure, chemically and physically, which is frequently analyzed by 3D ToF-SIMS technique. However, all of the complex intra-structure in OLED device should not be represented in 3D SIMS image due to the layer mixing by the differences of the sputtering yields.

In order to overcome this limitation, there are attempts in two ways: one is to perform topographic measurements by ex-situ technique such as atomic force microscopy (AFM), then manually combined with SIMS images with a suitable algorithm; the other is to integrate the in-situ SIMS-SPM instrument by SIMS manufactory [6–10].

In this work, we present a methodological development for combining the disparate images from SIMS and AFM, called to the 2D/3D data correlation in Fig. 1. To design the new algorithm, we've tried to add a concept: simplicity. In first, the algorithm has been employed the semiautomatic alignment system, which lead to reduce the effort to align the same measuring point when the data are

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