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A Complete Characterization of Samples Using Multivariate Statistical Analysis of 3Dimensional MCs^+ ToF-SIMS Data

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Depth profiling via Time of Flight Secondary Ion Mass Spectrometry (ToF-SIMS) is a well established technique that is used to determine the depth distribution of trace species in samples[1]. 3D depth profiling techniques are now being heavily utilized in the ToF-SIMS community since it enables the measurement of both the depth distribution and the lateral distribution of the species[2]. 3D ToF-SIMS analysis are revealing that many samples are not uniform in the lateral dimension[2]. Since a full mass spectrum is saved at every volume element, unexpected species are often found sub-surface, especially in real-world sample. Unfortunately, one often needs to perform two depth profile measurements in order to fully characterize a sample – a positive ion measurement to look for electropositive species with the highest sensitivity and a negative ion measurement in order to analyze electronegative species with the highest sensitivity. The two depth profile measurements are often performed using different erosion sources and experimental conditions which have been optimized for the species to be analyzed and often have significant differences in the erosion rate. Since the analysis are performed in two different regions of the sample, one can not correlate species observed in the two independent measurements. Additionally, there are instances where the amount of material is limited and one can not perform two measurements. MCs^+ analysis have been reported in the ToF-SIMS literature [3]. For MCs^+ analysis one uses a Cs ion beam to erode the sample, and a Bi_3 ion beam to perform the analysis in the positive ion polarity. Electropositive species are detected as M^+ and/or $M{+}Cs^+$ and the electronegative species are detected as M^+ and/or $M{+}Cs_2^+$ (where M is the element being analyzed). In this paper, we will demonstrate the ability to analyze complicated 3D MCs^+ ToF-SIMS data sets using multivariate statistical analysis (MVSA) techniques [2,4]. FIG 1 shows a color overlay of 8 MVSA derived component 3D images. FIG 2 shows a color overlay of the two interfacial components - images (top) and corresponding spectra (bottom). We will show the advantages of MVSA analysis over univariate analysis.

References

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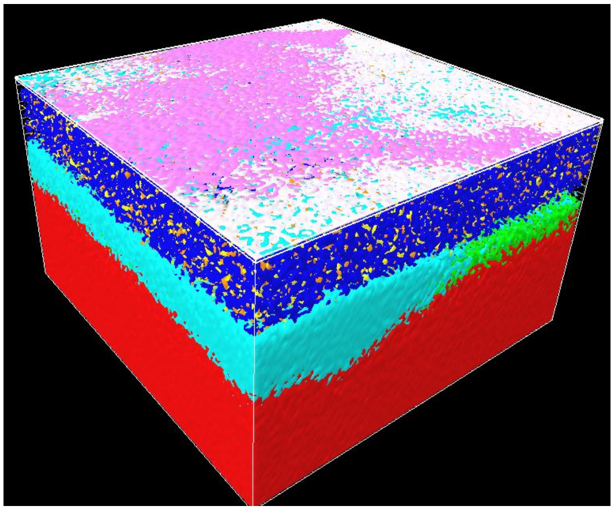

FIG. 1 Overlay of the eight MVSA component images: CZT substrate (red), CZT/gold interface – two components (light blue and light green), Au – three components (blue, orange, yellow), and surface contaminants – two components (white, pink).

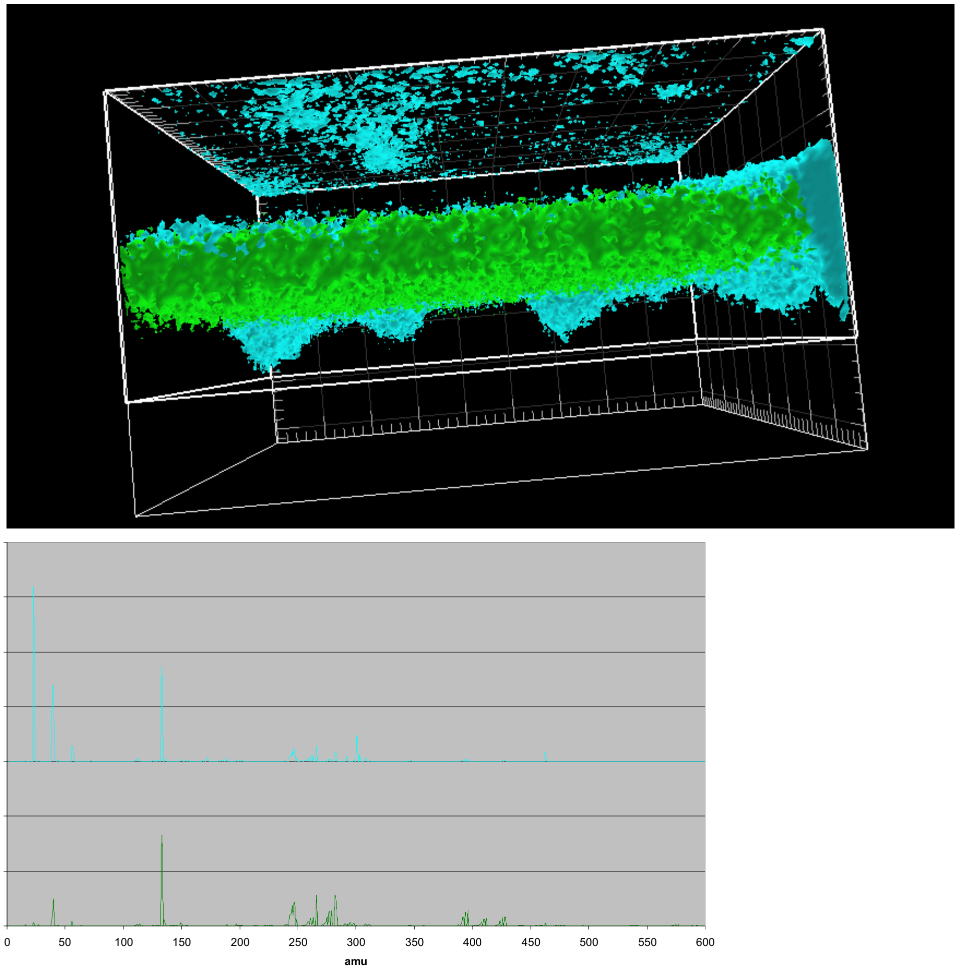

FIG 2. Color overlay of the two interfacial components; images (top) and corresponding spectra (bottom).