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Self-modeling Mixture Analysis of SIMS Image Data

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Introduction

The data analyzed in this study consisted of a two component mixture of stearic and palmitic acid, as schematically represented in Figure 1. Three drops were deposited on an aluminum foil substrate. The first drop contained palmitic acid and is indicated as A in Fig. 1. A second drop containing stearic acid is indicated as B. The third drop contained a 50/50 mixture of the components and is indicated as 0.5A+0.5B. The solvent was evaporated prior to analysis.

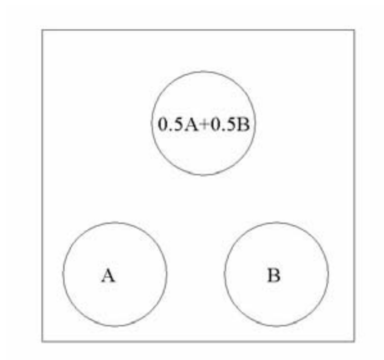

Figure 1. Schematic representation of the mixture sample analyzed with SIMS.

The sample was analyzed by an ION TOF IV time-of-flight secondary-ion mass spectrometer (TOF-SIMS).

The goal of this analysis was to resolve the image data into separate images of the pure components and their associated mass spectra.

Results and Discussion

With self-modeling imaging techniques such as the functions `purity`, `ALS`, and `MCR`, the data can be resolved in four images (Figure 2). Images 1 and 2 represent the background caused by a coating on the aluminum foil. Images 3 and 4 represent the properly resolved images of palmitic acid and the stearic acid. It is clear that the sample spot with a mixture of the two components was properly resolved, since it is visible on both images 3 and 4.

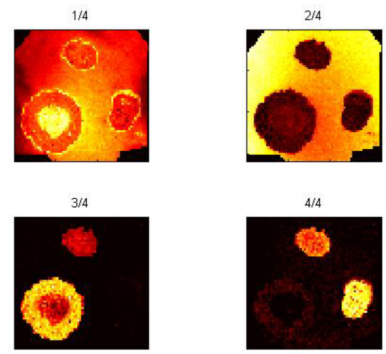

Figure 2. The resolved images. Images 1 and 2 represent the coating on the aluminum foil, image 3 represents palmitic acid and image 4 represents stearic acid.

Figure 3 shows raw spectra from the original data representing palmitic acid (spectrum 1) and stearic acid (spectrum 2). The palmitic acid spectrum is characterized by m/e 257 (M+H) and 239 (M+H-H_20) and the stearic acid by 285 (M+H) and 267 (M+H-H_20). In addition to palmitic acid and stearic acid, there are contributions from the aluminum foil coating in the lower mass range. Spectra 3 and 4 are resolved spectra of palmitic acid and stearic acid resulting from the self-modeling mixture analysis. We see that the contribution from the background signature is significantly lower than in the raw spectrum.

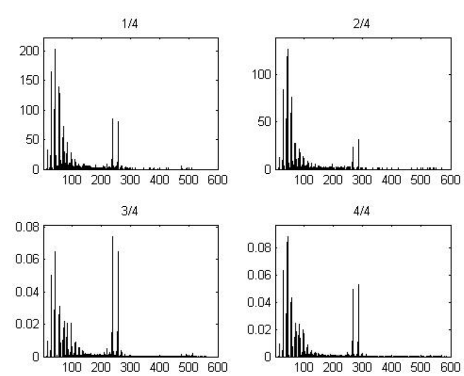

Figure 3. Spectra 1 and 2 are from the palmitic and stearic acid samples in the original data set. The resolved spectra 3 and 4 clearly show a more prominent signal of palmitc acid (spectrum 3) and stearic acid (sample 4).

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Conclusion

This example shows that it is possible to effectively resolve images from SIMS data of mixtures. The success of the resolution process is clear from the resolved spectra of palmitic and stearic acid, which clearly show reduced contribution from the aluminum foil background in the lower mass range. The resolved images in Figure 2 confirm the successful resolution.

Literature

1) Y. Batonneau, J. Laureyns, J.C. Merlin, C. Bremard, Self-modeling mixture analysis of Raman microspectrometric investigations of dust emitted by lead and zinc smelters, Anal. Chim. Acta, 446, 2001, 23-37.