

Extended Abstract of PSA-19

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Analysis of TOF-SIMS and microscope fused image data using sparse modeling and deep learning

Satoka Aoyagi,^{1,*} Tomomi Akiyama,¹ Takayuki Yamagishi¹

¹ Faculty of Science and Technology, Seikei University, 3-3-1 Kichijoji-Kitamachi, Musashino-shi, Tokyo 180-8633 Japan

* aoyagi@st.seikei.ac.jp

(Received: May 29, 2019; Accepted: July 01, 2019)

Image data fusion of time-of-flight secondary ion mass spectrometry (TOF-SIMS) and scanning electron microscopy (SEM) data was investigated. The fused data were analyzed with multivariate analysis, deep learning, and sparse modeling to study what types of information could be extracted from data analysis. Image fusion with a method having higher spatial resolution provides not only higher resolution images but also more detailed chemical information. Microscope images could be useful guides to classify the samples and extract region of interest even if it is unknown. Model samples having micro meter patterns were analyzed by TOF-SIMS and SEM or optical microscopy. The same sample areas were trimmed from image data obtained with different methods and then fused by adding the other one's intensity at each pixel to TOF-SIMS peak intensities. The patterns in the sample observed with SEM are helpful to extract important secondary ion information with reduced influence of noises. LASSO (least absolute shrinkage and selection operator) and Autoencoder, one of the deep learning techniques, extracted main information of the model samples as well as principal component analysis (PCA).

1. Introduction

Time-of-flight secondary ion mass spectrometry (TOF-SIMS) is one of the most powerful chemical imaging techniques because it provides high spatial resolution, such as 100 nm lateral resolution and several nm depth resolution, images of ions produced from a sample. However, higher spatial resolution is often required when samples having nano-structures such as biological cells and intelligent devices. The spatial resolution of TOF-SIMS could be increased by appropriate data analysis applications such as noise reduction, multivariate analysis, sparse modeling and deep learning. Image fusion of TOF-SIMS and other methods providing higher spatial resolution is a promising technique as well. The image fusion of several surface analysis techniques such as TOF-SIMS and scanning electron microscope (SEM) has been recently reported [1,2]. In this study, fundamental investigations for effective image fusion to TOF-SIMS and microscopic techniques were studied to develop a standard process for image fusion for chemical imaging

techniques. Model samples were AFM standard sample which has five-micro-meter patterns and biological cells.

2. Materials and Methods

2.1 Sample

The schematic of AFM standard sample (SU134-20, EM Japan Co.) is shown in Fig. 1. The 1 × 1 mm square standard sample has patterned layers of SiO₂ (the thickness is 20 nm) on a Si substrate as shown in Fig. 1. There are small cubes, holes and lines of SiO₂ (5 μm pitch) in 500 × 500 μm square in the center of the sample and the pitch of the cubes and holes outside of the center square is 10 μm.

2.2 TOF-SIMS and SEM

The AFM standard sample was measured with TOF-SIMS (TRIFT III, ULVAC-PHI, Chigasaki) with 22 keV Au⁺ (Raster size; 100 × 100 μm² or 300 × 300 μm², Pixel density; 256 × 256 pixels) and a scanning electron microscope (SEM, S-3400N, Hitachi, Ltd., Tokyo) of accelerating voltage; 1.5 kV, emission current; 40 mA and working distance; 5 mm.

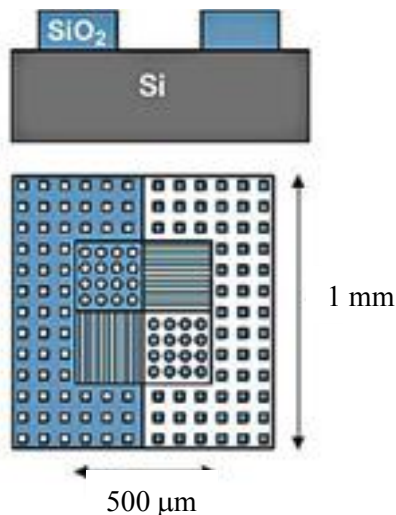


Fig. 1 Schematic of AFM standard sample (SU134-20). The sample has 5 μm pitch patterns of SiO_2 on Si substrate.

2.3 Image Data Fusion

A secondary ion image of TOF-SIMS was fused with a grey scaled SEM image. TOF-SIMS image resolution was aligned to the microscopic image resolution to make these two images have the same resolution, (e.g. 128×128). Intensity subtraction between TOF-SIMS and microscopic images at each pixel was obtained and then the total of the subtraction was calculated. This process was repeated with a slightly different microscopic image trimmed from the original data until the minimum total subtraction was obtained. In the image fusion data, microscopic image information was added to one of the variables (second ion peaks) of TOF-SIMS data. The image fusion data was analyzed by PCA (principal component analysis) using the PLS Toolbox (Eigenvector Research Inc., WA, USA) for Matlab (Mathworks, MA, USA) and Autoencoder [Deep Learning Toolbox, Matlab, Mathworks]. The TOF-SIMS data was also analyzed using one of the sparse modeling methods, LASSO (least absolute shrinkage and selection operator) [3, 4]. In LASSO, the grey-scaled SEM data was used as a solution y of the following equation:

$$y = Ax + \text{noise}$$

where matrix A is the TOF-SIMS data and x is a vector representing the spectra equation which extract spectra, out of the TOF-SIMS data A , corresponding to y . Suppose the noise is so small that the noise can be ignored. LASSO searches x which makes $E(x)$ minimum.

$$E(x) = \|y - Ax\|^2 + \lambda \sum |x_i|$$

where λ is a hyper-parameter depending on the importance of sparsity for the data A .

3. Results and Discussion

The same region was extracted from SEM and TOF-SIMS data by comparing each pixel intensity. If the two figures are completely the same the total subtraction of each pixel should be 0. Trimming areas are changed until the minimum pixel subtraction. The SEM image was rotated until the minimum pixel subtraction.

As a result, SiO_2 related secondary ions, such as m/z 60.98 (SiO_2H^-) and m/z 59.96 (SiO_2^-), are directly indicated by LASSO and Autoencoder.

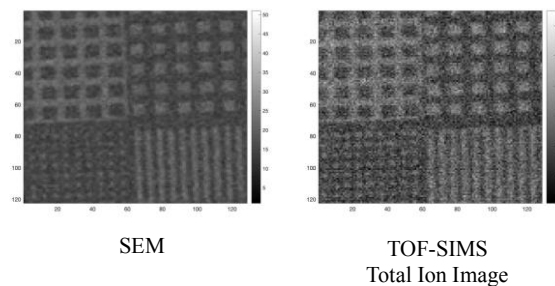


Fig. 2 SEM and TOF-SIMS total ion images for image data fusion.

4. Conclusions

The image fusion of images by two surface analysis methods provides more detailed information than what each method could provide. Some of the data analysis techniques which have already been applied to other fields such as Autoencoder (deep learning) and LASSO (sparse modeling) are useful for extracting important information from the fused data, which is not always found by manual analysis.

5. References

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