Gigapixel X-ray micro-spectroscopy data analysis by using machine learning

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Multi-scale analysis techniques from the nanoscale to the macroscale are essential to understand the correlation between the structure and properties of materials. We developed a gigapixel X-ray microscope (G-XRM) realizing a high resolution and an ultra-wide field of view simultaneously. As a result, we obtained X-ray absorption spectra (XAFS) in the field of view of the centimeter scale with spatial resolution on the nanometer scale.

Since the number of acquired spectra can reach 0.1 to 1 billion, machine learning is essential to analyze the big data. The aim of this study is clustering by chemical states. A method of chemical state clustering of TXM measurement data (0.3MPixels) by spectral similarity has been reported [1]. Methods reported so far treat each pixel spectrum independently. However, the dataset may contain the spatial information as well: neighboring pixels are more likely to take the same chemical state. Therefore, we developed a clustering method for a large-scale spectral data set that utilizes a standard spectral database [2-3] to calculate spectral similarity and an image processing approach to integrate spatial information. Moreover, we evaluated this method.

We measured Fe-K edge XAFS for sintered ore whose chemical state is unknown and heterogeneous by using G-XRM, and we got 450M spectra with a spatial resolution of about 500 nm. Figure 1 shows the visualization results of chemical states by the proposed clustering method. The results revealed the existence of a previously undiscovered phase in the sintered ore. SEM-EDX measurements in the region confirmed that we have succeeded in finding a new chemical state that had been missed using conventional methods.

This method enables high-resolution and ultra-wide-field observation of chemical states without prior knowledge and, for example, is expected to understand the chemical reactions in battery materials.

![Figure 1](image.png)

**Figure 1.** Chemical state clustering from 450M XAFS data with about 500 nm spatial resolution


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