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High Accuracy EDS Chemical Mapping Using High Speed Clustering Analysis

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Multivariate analysis, such as principal component analysis (PCA) is used for producing EDS chemical mapping. The PCA is simple for classifying main components, however, may be unsuitable for trace components. Therefore, we tried to speed up agglomerative hierarchical clustering (AHC) by using self-organizing map (SOM). As a result, we confirmed that our high speed clustering analysis (HSCA) can classify components which not classified by the PCA.

The HSCA performs a cluster analysis of the EDS spectrum cube, and produces a chemical map based from the clustering result. The HSCA executes two steps. In the first step, SOM makes a few tens clusters from all spectra. These clusters are used as initial clusters of AHC for the second step. In the normal hierarchical clustering, the computational effort becomes enlarged with the number of data because the calculation order of hierarchical clustering is $N^2\log(N)$. In order to reduce this order, we reduce the number of data to several tens by using SOM. Therefore, the HSCA is much faster than normal hierarchical clustering.

The HCSA was tested by using mixture of five type glasses (PA4, PB2, PD3, PE3 and PF3, provided from LGC Standards) embedded by epoxy. Figure 1 shows a secondary electron image of the test sample (a) and a spectrum of each glass (b). The glasses are mainly classified two groups, SiO_2-rich (PA4, PB, PE3 and PF3) and Al_2O_3-rich (PD3). In addition, the minor components such as Na_2O, MgO, K_2O and CaO are different for each glass. Figure 2 compares chemical maps produced by PCA, and HSCA. The EDS spectrum cube was taken at Acc. Vol. 20 kV. The image resolution was 256 x 192 pixels. The number of components was set to eight which was estimated from a scree plot of the initial clusters of AHC. The PCA could classify PB2 (red), PF3 (green) and epoxy (orange), but could not distinguish PA4, PD3 and PE3 (light pink). Other components (blue, yellow, magenta and white) were assigned to noise and a few edges caused by the electron diffusion. It means that the PCA might miss to classify the miner elements because the PCA focuses only some major elements. The HSCA could classify PA4 (magenta), PB2 (red), PD3 (yellow), PE3 (light pink) and PF3 (green). Moreover, the epoxy had two components of white and orange. The orange had re-deposited contaminants caused by the cross section polishing process. The remaining component was the edge (blue). It means the HSCA can classify spectra containing trace elements. Therefore, the HSCA can produce chemical maps closer to human judgment than the PCA.

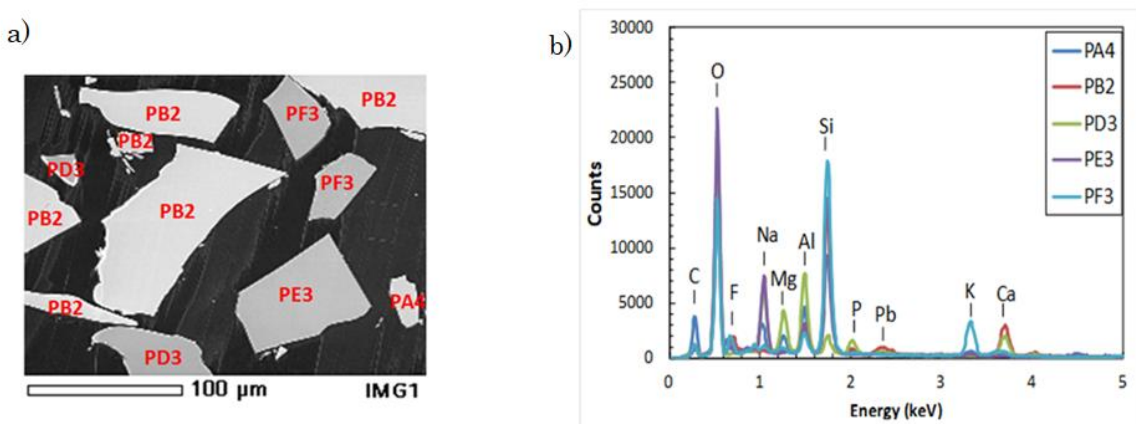

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Figure 1. The secondary electron image of the glass powder mixture (a) and X-ray spectrum of each glass (b).

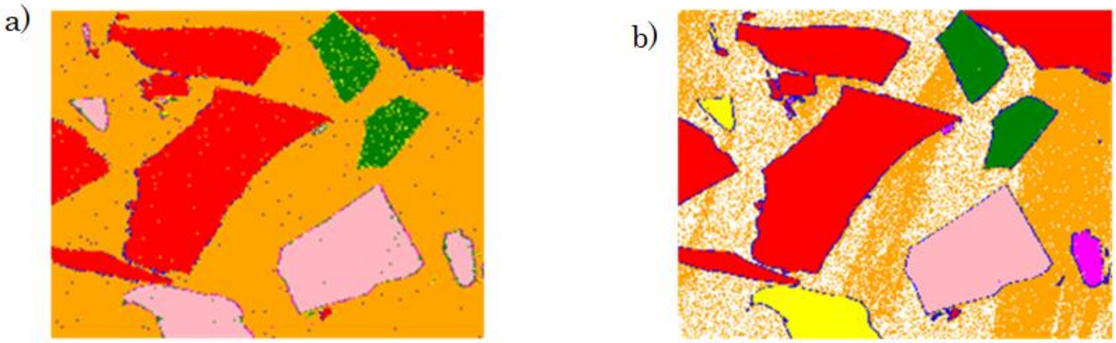

Figure 2. The chemical map produced by the PCA (a), and the HSCA(b).

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