EDS Chemical Mapping by Unmixing of Spectral Imaging Data

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Abstract

EDS chemical mapping is a method to visualize equivalent chemical composition areas by classifying spectra in spectral imaging data (SI). Classification of large numbers of spectra, hundreds of thousands or even more, can be achieved by machine learning.

However, hard clustering methods provide a map filled with homogeneous colors, even in the areas with the inhomogeneous compositions. Non-negative Matrix Factorization (NMF), one of the spectral decomposition method, can represent gradual changes of spectra as continuous changes in the abundance of components. On the other hand, the components may converge to unnatural results as an EDS spectrum.

In this work, we tried to create EDS chemical map by unmixing SI with the most characteristic spectra extracted from the SI by Vertex Component Analysis (VCA)[1].

As a result, we obtained the chemical map that not only could represent gradual changes in composition, but also gives easier understanding of the chemical composition.

1. Sample for the Verification

Polished section of chondrite meteorite – contains 10 substances (phases)

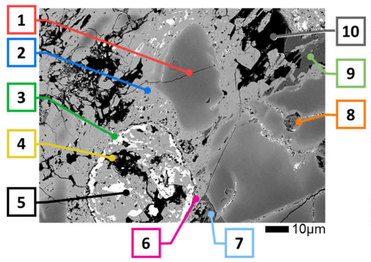

Fig.1: The backscattered electron image of the sample.
There are various kinds of minerals such as olivine (1,2), apatite (4), and Fe-Ni metal (5) .

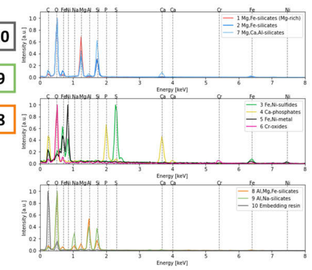

Fig.2: X-ray spectrum of each area.
Compound name in the legend are based on the quantitative analysis results.
Acc. Vol. 10 kV.

Complicated texture, Zoning and Small grains

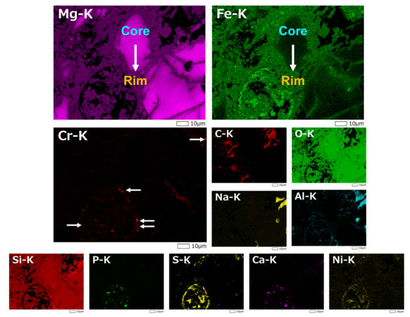

Fig.3: The elemental maps of the sample.
Cr is sparsely located, as indicated by arrows.
Acc. Vol. 10 kV. EDS map size: 256x192 pixels.

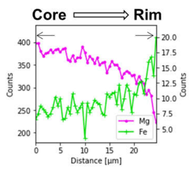

Fig.4: The X-ray intensity of Mg and Fe in the grain at the center.
The X-ray intensity of Mg (pink, dot) and Fe (green, cross) from core to rim showing the gradual changes seemingly due to zoning.

2. Chemical mapping by Cluster analysis

Process:

1. **Preprocess**
   1. Emphasize features in spectra.
   2. Convert each spectrum to intensities at major peak.
2. **Agglomerative Clustering**[2]
3. **Drawing Chemical map**
   Fill pixels linked to clusters.
4. **Identify chemical composition**
   Qualitative analysis of averaged spectrum from each cluster.

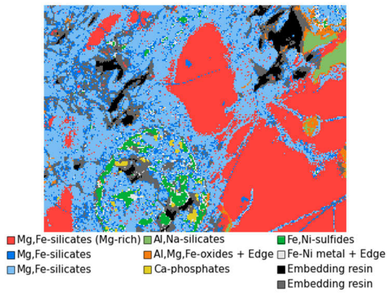

Fig.5: The chemical map by Cluster analysis.
Monochromatic red was used for zoning areas. The small grains of Cr-oxides could not be distinguished, while the embedding resin and Mg, Fe-silicates were separated into two clusters, respectively.

Results:

- **Indicate Zoning >> Not**
  Cluster analysis does not support overlap, which means belonging to more than one cluster.
- **Small grains of Cr-oxides >> Not distinguished**

3. Chemical mapping by NMF

Process:

1. **Preprocess**
   Emphasize features in spectra.
2. **NMF** (Non negative Matrix Factorization)[3]
   Convert SI into several components and its abundance.
3. **Drawing Chemical map**
   Overlay the abundance maps.
4. **Identify chemical composition**
   Qualitative analysis of components while ignoring dips.

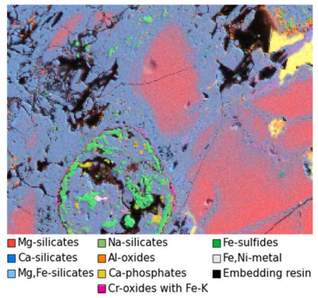

Fig.6: Chemical map by NMF.
The center grain was represented by a gradual color change from the red (Mg-silicates) to light blue (Mg, Fe-silicates). The small grains of Cr-oxides were marked with pink.

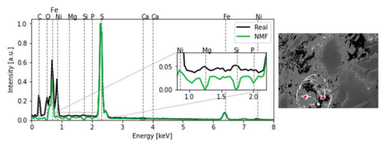

Fig.7: The NMF component and real EDS spectrum corresponding to Fe, Ni-sulfides.
NMF (green): showing dips at characteristic X-ray energy of O, Mg, Si, and Ca, which are unnatural for EDS.
Real (black): created by integrating the spectra in the red rectangle areas indicated on the BSE image.

Results:

- **Indicate Zoning >> Done**
  As changes in the abundance of the components.
- **Small grains of Cr-oxides >> Distinguished**
- **Understanding chemical composition >> Not easy**
  Due to dips and inconsistency of peaks (K line peaks but no L line peaks).

4. Chemical mapping by VCA

Process:

1. **Preprocess**
   Emphasize features in spectra.
2. **VCA** (Vertex Component Analysis)[3]
   Find vertex spectra.
3. **Drawing Chemical map**
   Overlay the projections of the vertex spectra.
4. **Identify chemical composition**
   Qualitative analysis of the vertex spectra.

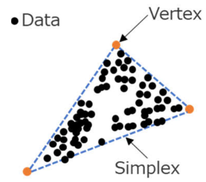

Fig.8: Conceptual Diagram of VCA.
VCA is an algorithm that finds the vertices from simplex-shaped dataset. The vertices of SI can be used for unmixing SI by its own signature spectra.

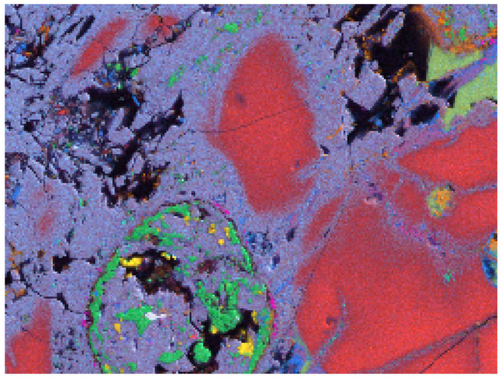

Fig.9: Chemical map by VCA.
The center grain was represented by inhomogeneous red (Mg, Fe-silicates). The small grains of Cr-oxides were indicated with pink.

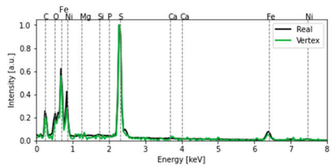

Fig.10: The vertex spectrum and real EDS spectrum corresponding to Fe, Ni-sulfides.
Vertex spectrum (green): obtained by VCA.
Real (black): same as real EDS spectrum in Fig.7.

Results:

- **Indicate Zoning >> Done**
  As projection images of vertex spectra.
- **Small grains of Cr-oxides >> Distinguished**
- **Understanding chemical composition >> Easy**
  Vertex data are the real EDS spectra exist in the SI.

Summary

We tried to create a chemical map by unmixing SI using the most characteristic spectra extracted from the SI by VCA.
In this work, the EDS spectral imaging data containing zoning area, showing gradual change of composition was used.
Although the areas were represented as if they have homogeneous composition in the cluster analysis based map, NMF and VCA could indicate them by using inhomogeneous colors. In terms of identifying the chemical composition of each area, the VCA based map was more practical than NMF.
We hope the method can be applied to and help various kinds of field of research.

Acknowledgments

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Reference

[1] J. M. P. Nascimento and J. M. B. Dias, IEEE TRANSACTIONS ON GEOSCIENCE AND REMOTE SENSING 43(2005), p.898. doi:10.1109/TGRS.2005.844293
[2] Scikit-learn: Machine Learning in Python, Pedregosa et al., JMLR 12, pp. 2825-2830, 2011.
[3] GitHub - MotokiShiga/malspy: Machine Learning for Spectral Imaging, https://github.com/MotokiShiga/malspy (October 22,2022)