Goldschmidt 2026 Abstract
https://doi.org/10.46427/gold2026.37692

Machine Learning Analysis of XANES Observations of Ryugu Return Samples

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Studies of organic matter in samples collected from asteroid 162173 Ryugu demonstrate a wide variety of carbonaceous material, both similar to that found in CI chondrites and either rare, or unreported, in CI chondrites, all consistent with the pristine nature of the sample. We combine x-ray absorption near-edge structure spectroscopy (XANES) with machine learning to search for unreported instances of pristine carbonaceous phases in Ryugu samples and possible spatial relationships to mineral phases.

XANES spectra for C, N, O, Ca, and Fe (e.g., Fig 1A) were collected for multiple sections from two Ryugu particles. Traditional data analysis methods were compared with autoencoder machine learning analyses of combined C, N, and O spectra (Fig. 1B). Autoencoder results were reduced using a K-means (n=9) clustering algorithm to identify phases based on autoencoded representation of the spectra. The number of clusters was set to be the minimum number of clusters required to distinguish known magnetite grains (Fig. 1C) from the surrounding matrix. Clustering revealed multiple N-rich regions which were not initially identified by eye. These regions are similar to a highly N-enriched grain, initially identified by eye, present in A0108-11-1 which exhibits a C-XANES peak at 285.0 eV in addition to broad a C-XANES peak at 286.5 eV and a distinct N-XANES amide ($CONH_x$) peak at 401.2 eV (Fig. 1D). N-rich regions all exhibit the characteristic peak at 401.2 eV not present in other regions (Fig. 2). The high N-rich grain observed A0108-11-1 represents a new type of organic matter in Ryugu for which we find no matches in the literature. The C peak at 285 eV indicates aromatic C=C, while the broad C peak at 286.5 eV in conjunction with the N peak at 401.2 eV indicates significant amide functional groups.

9 clusters are sufficient to separate certain phases, expected phases (e.g, IOM-like, highly aromatic, and molecular carbonate “hotspots”) are incorporated into the current phases due to lower-order differences in their spectra. Further analyses incorporating a greater number of clusters alongside TEM data will allow us to distinguish such phases.

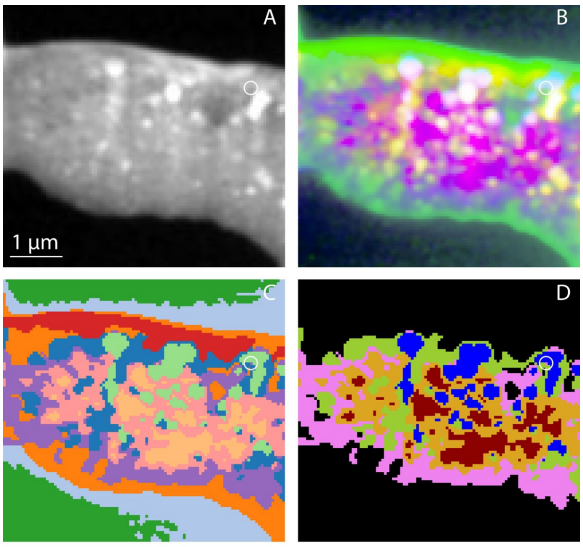


Figure 1: A) 285 eV XANES image of Ryugu sample A0108-11. B) Result of autoencoder analysis with pixels of like color indicative of similar spectral features. C) K-means clustering (n=9) of autoencoder output. D) K-means clustering reduced to discrete phases based on cluster average spectra (e.g., magnetite = blue, N-rich = maroon, pink) circle represents where N-rich grain was found by manual inspection of spectra.

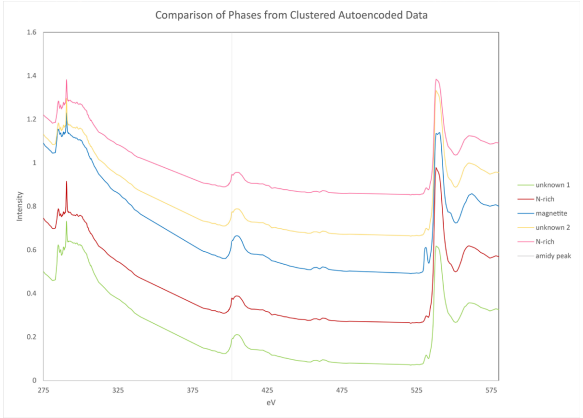


Figure 2: Average spectra for phases as identified by K-means clustering algorithm (n=9). Two N-rich phases are present with strong amidyl peaks at 401.2 eV. Magnetite is identified by the characteristic double peak at 538 eV.