Spectral-Spatial Mineral Classification Using EDS X-ray Images: Application to Shergottites

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Motivation

Modern instrumentation allows the collection of very large data volumes of chemical microanalytical data in the form of X-ray chemical maps using scanning electron microscopes equipped for energy dispersive X-ray spectroscopy (EDS). A typical EDS data set for a petrographic thin section might produce ten or more images of several mb, imaging an area of a few cm² at a resolution of a few µm/pixel. Thus, it is rapidly becoming practically impossible for a human investigator to carefully examine the full data set. The EDS data set provides a rich set of features to identify minerals in a thin section using machine learning. Supervised learning algorithms enable an expert to manually identify a small representative sample of minerals and apply that classification to the entire image. Reliable classification can form the basis of further qualitative and quantitative analyses, and provides useful insights when the classes can be assigned physical meaning (e.g., in terms of minerals).

NWA 7257 Image Data

Northwest Africa 7257 is an enriched shergottite consisting dominantly of elongate euhedral to subhedral pyroxene laths (containing a mixture of pigeonite, augite, and ferroaugite) with interstitial plagioclase (Table 1). Accessory phases include ilmenite, Fe-Cr-Ti spinel, pyrrhotite, chlorapatite, maskelynite, K-rich melt pockets, and rare baddeleyite and fayalite [1].

Supervised electron (BSE) imagery & EDS X-ray spectra were acquired for a polished thin section of NWA 7257 using a JEOL JSM-7001F scanning electron microscope with Oxford Emax detector. The X-ray spectra were sampled to produce images which map the intensity of individual elements (Al, C, Ca, Cl, Cr, Fe, K, Mg, Mn, Na, O, P, S, Si, Ti, Zr).

Classification Strategy

This approach adapts the technique proposed by Tarabalka et al. [2] for classifying hyperspectral satellite images. A flowchart of the algorithm is shown to the right.

Spectral Classification

The initial step uses a support vector machine (SVM) to perform a probabilistic classification for every pixel in the image. The SVM learns from the training data by dividing the N-dimensional feature space into k sub-regions by maximizing the margins between the classes. Each pixel of the image is mapped to one of the k sub-regions to obtain the spectral classification map.

Spatial Regularization

The spectral classification considers only the information available at each pixel location. Most structures in the image are larger than one pixel. The SVM does not take the spatial structure of the data into account, which results in a noisy classification map. A Markov Random Field (MRF) regularization step is used to smooth the result. This approach is based on the assumption that a pixel belonging to a given class is likely to be surrounded by pixels having the same class. The regularization is formulated as the minimization of a suitable energy function.

The energy function of a pixel x has a spectral component and a spatial component:

\[ E(x) = E_{\text{spectral}}(x) + E_{\text{spatial}}(x) \]

The spectral energy term is:

\[ E_{\text{spectral}}(x) = -\ln P(x|L) \]

The spatial energy is found by comparing the class of a pixel with the class of its neighboring pixels. For pixel x, let η denote the set of η immediately neighboring pixels. The spatial energy is calculated by:

\[ E_{\text{spatial}}(x) = \sum_{\eta(x)} \theta(1 - \delta(L_x, L)) \]

A Metropolis algorithm [3] is employed to stochastically relax the global spectral/spatial energy. This is an iterative algorithm that randomly selects a pixel, and randomly selects a new class. If the new class would lower the energy of that pixel, it is assigned. Otherwise, it may still be assigned with a probability that decreases over time.

Results and Discussion

The final result clearly distinguishes many key petrographic features including the pigeonite cores of pyroxene laths, complex augite and ferroaugite overgrowths, and interstitial maskelynite and melt. The regulated classification provides a useful dataset for further quantitative analysis. The regulated classification results by comparison with measurement data.

Future Work

Validation of classification results by comparison with measurement data.

References