Classification of minerals using nonlinear correlation of Raman Spectrum data

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ABSTRACT:
In this work a methodology to recognize minerals by using only phase information of the vectors, obtained for both the target and the problem spectrum vector, is used. In many classification problems of signals and automatic detection of objects, it is necessary to search in spectral database in order to identify objects to make decisions. This algorithm is computationally inexpensive and thus susceptible to be used like a part of the new information technology devices in the field of portable spectrometry or automatic scanning, particularly in the area of the mineralogy and crystallography because the nature of the spectra are of the type Raman.

Key words: Spectral image recognition, nonlinear correlation, spectral signatures, Fourier transform.

REFERENCES AND LINKS

1. Introduction
In applied physics including digital optics and geosciences is necessary to build efficient data processing equipment to make use of algorithms for pattern recognition to detect objects or chemical compounds in spectrometry of minerals [1], with low cost computational, which is one of the main requirements in an automated computer vision scanning using autonomous machines[2-3]. In this work a method to classify different kind of minerals by using identity vectors signatures of spectra minerals is used. To facilitate the automatic identification of patterns in minerals, information from optical spectrometry useful for identification of different objects which has proved to be useful in pattern recognition is used. The algorithm uses non linear correlation applied to the identification of spectra minerals in a set of spectra, which can be extended to searches in a spectral database of N records.

2. Methodology
The procedure used in this work uses the phase of the reference data and is compared with the phase only of the data or vector of the mineral to be recognized. The nonlinear correlation can be expressed like

\[ C_{NL} = S^{-1} \left[ \exp[i\phi] \cdot \exp[-i\phi] \right], \]  

(1)
where \( \phi \) is the phase of the vector of the mineral to be classified, \( \phi \) is the phase of the mineral reference vector and \( \mathcal{F}^{-1} \) is the inverse Fourier transform.

2. a Identity vectors signatures.
The mineral to be recognized is denoted by \( f(x) \) which is a vector representation or the Raman spectrum of the mineral (Fig. 1). Each mineral is represented by a unique Raman spectrum.

![Adamite Raman spectrum](image)

Fig. 1 Example of Raman spectrum of the mineral from RRUFF database

3. Results.
To evaluate the performance of this computational system, 10 test Raman spectra of different materials were used and downloaded from RRUFF project. The results for different instances of records used to recognize a spectrum target have a confidence level above 95.4% in all the cases. Each Raman spectrum used in the classification could be recognized above this confidence level.

4. Conclusion.
The system presented is an excellent alternative for the development embedded software in hardware vision devices for automatic recognition of spectra in site where the samples and information is processed. This work is addressed in the direction of applying the new information technologies to the traditional ways of processing information in important areas such as pattern recognition in mineralogy, particularly for the development of portable detection instruments that require autonomous high performance and low computational costs that allows the analysis at the site of the objects, allowing the identification and characterization of the environment immediately surrounding the sampling area.

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