Computers & Geosciences 54 (2013) 259–268

Contents lists available at SciVerse ScienceDirect

Computers & Geosciences

journal homepage: www.elsevier.com/locate/cageo

An automated mineral classifier using Raman spectra

Sascha T. Ishikawa [a,b,*], Virginia C. Gulick [a,c]

[a] Space Sciences Division, NASA Ames Research Center, MS 239-20, Moffett Field, CA 94035, United States
[b] University of California Santa Cruz, Santa Cruz, CA 95064, United States
[c] SETI Institute, 189 Bernardo Avenue, Mountain View, CA 94043, United States

ARTICLE INFO

Article history:
Received 2 September 2012
Received in revised form
26 January 2013
Accepted 29 January 2013
Available online 5 February 2013

Keywords:
Mineral classification
Raman spectroscopy
Machine learning
Mars
Robotic exploration
Igneous rocks

ABSTRACT

We present a robust and autonomous mineral classifier for analyzing igneous rocks. Our study shows that machine learning methods, specifically artificial neural networks, can be trained using spectral data acquired by in situ Raman spectroscopy in order to accurately distinguish among key minerals for characterizing the composition of igneous rocks. These minerals include olivine, quartz, plagioclase, potassium feldspar, mica, and several pyroxenes. On average, our classifier performed with 83 percent accuracy. Quartz and olivine, as well as the pyroxenes, were classified with 100 percent accuracy. In addition to using traditional features such as the location of spectral bands and their shapes, our automated mineral classifier was able to incorporate fluorescence patterns, which are not as easily perceived by humans, into its classification scheme. The latter was able to improve the classification accuracy and is an example of the robustness of our classifier.

1. Introduction

The characterization of geological features provides insight into the history and formation of a site. This process requires the following: (1) detailed morphological, physical, and compositional analyses of rocks and sediments within stratigraphic layers, units, outcrops, and landforms, and (2) the integration of this information into conceptual models used to unravel a region's geologic history. Unfortunately, exploring some geological sites may be difficult or even dangerous, as in the case of deep-sea hydrothermal vent studies on Earth, or in the remote exploration of the surface of Mars. As a result, these kinds of missions would benefit from assistance, or even full autonomy in the form of robotic explorers capable of performing onboard scientific analyses.

A key task in characterizing the geology of site is selecting which rocks and sediments to analyze. Our efforts to facilitate this process are towards developing technology to serve as a field assistant for geologists, as well as to equip robotic explorers with the capacity to perform unassisted compositional analyses of geologic samples.

In this paper, we provide an application of machine-learning techniques to create an automated classifier to estimate the presence of key minerals based on in situ Raman spectroscopy. We demonstrate the robustness of our method by using different sources of Raman spectral data, both from our own rock and mineral database, and from a third-party mineral database.

1.1. Raman spectroscopy

Raman spectroscopy provides a quick and non-invasive technique (Lewis and Edwards, 2001) to determine the mineral compositions of rocks and sediments. Samples are scanned with a laser without the need for preparation, such as grinding or pulverizing. Therefore, this approach enables the ability to analyze samples as they are found, without moving or altering them.

Raman spectroscopy works by directing a focused monochromatic light source at the surface of a mineral causing individual photons to scatter. Most of the photons will bounce off elastically with a negligible transfer of energy, a phenomenon known as Rayleigh scattering. However, a small portion of photons will be scattered inelastically with a corresponding transfer of energy between the photon and the mineral surface. The latter is called Raman scattering and is observed as a shift in wavelength between the incident light and the scattered light, which is recorded by a detector. The Raman shift occurs because energy from the incident photons is transformed into vibrational and rotational motions of surface molecules. Moreover, this shift in wavelength reveals important information about the molecular structure of minerals and it often provides a unique signature of the material being analyzed (Lewis and Edwards, 2001). The resulting "fingerprint" spectra enable us to automate the

* Corresponding author at: NASA Ames Research Center, Space Sciences Division, Mail Stop 239-20, Moffett Field, CA 94035, United States.
Tel.: +1 415 595 4996.
E-mail address: Sascha.T.Ishikawa@nasa.gov (S.T. Ishikawa).

0098-3004/$ - see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.cageo.2013.01.011

process of classifying minerals by using machine learning algorithms that exploit the uniqueness of such signatures.

1.2. The minerals

The presence of certain key minerals reveals important compositional information for determining the geologic origin of a rock. The minerals we used in this study help to discriminate between felsic and mafic igneous rocks. Mafic igneous rocks contain higher percentages of the minerals biotite, olivine, pyroxene, amphibole, and plagioclase feldspar than their felsic counterparts. Therefore, they are enriched in iron, magnesium, calcium and sodium, but are lower in silica. In contrast, felsic igneous rocks contain higher percentages of the minerals quartz, muscovite, and potassium feldspars and are thus enriched in silica, aluminum, and potassium.

A single mineral is often a subset of a larger mineral group. Individual minerals in a group, while different in their exact structure, may share a common chemical formula. For example, microcline ($KAlSi_3O_8$) is a lower temperature polymorph of orthoclase; although it has the same chemical formula, it possesses a different structure. Both are potassium-rich alkali feldspars, or *K*-spars. Minerals in the plagioclase group have a general chemical formula (Na, Ca)$Al_{1-2}Si_{2-3}O_8$ where the amounts of aluminum and silicon vary based on which end member (Na or Ca) is present. These minerals range from a sodium-rich albite ($NaAlSi_3O_8$) through oligoclase, andesine, labradorite, bytownite, and calcium-rich anorthite ($CaAl_2Si_2O_8$). A similar relationship extends to the remaining mineral groups considered in this study. The shared characteristics among minerals carry over to their spectral signatures, which in some cases are virtually indistinguishable in terms of individual spectra. See for example, microcline versus orthoclase in Fig. 1. Based on this ambiguity, we would expect poor resolution between certain minerals in our classifier. Instead, we find that our classifier is able to distinguish between some minerals despite the remarkable similarities in their spectra. Fig. 1 illustrates the spectral profiles of all six mineral groups considered in this study. Each individual curve represents an average of ten normalized spectral observations of a mineral specimen from the training set.

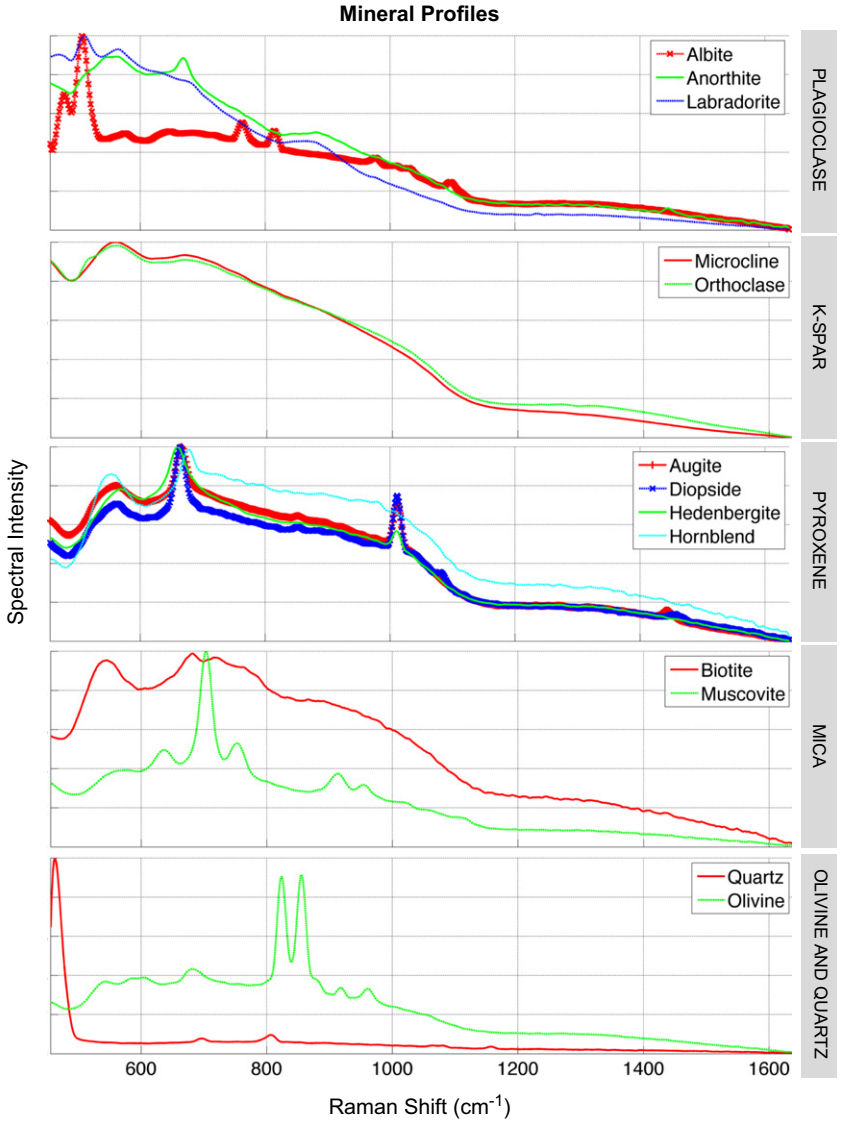

Fig. 1. Typical mineral spectra from our collection used in this study. Each plot was obtained by averaging all spectral observations for each mineral type, normalizing the spectral intensity values to the range [0,1], and smoothing with a Savitzky–Golay filter. The plots show the Raman bands associated with specific mineral groups as well as their broader fluorescence bands.