Using LIBS for classification of carbonate minerals on Mars

Abstract

The first laser-induced breakdown spectroscopy (LIBS) instrument for extraterrestrial applications will be used onboard the NASA Mars Science Laboratory (MSL) Rover 'Curiosity,' scheduled for launch in 2011. Researchers at Los Alamos National Labs and the University of New Mexico are using LIBS to understand the chemical composition of rocks, determine if they can classify the rocks, and deduce information about the presence and amount of water on Mars. LIBS data will be collected by the Rover at a distance of up to 7 meters from the Martian samples, and multivariate data analysis will be used to classify the rocks based on their composition.

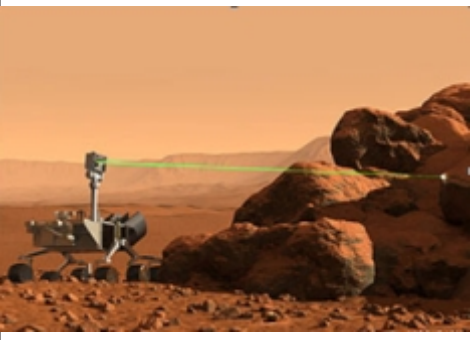

Figure 1: *Depiction of Mars Rover with ChemCam*

Introduction

LIBS is a powerful technique for determining the elemental composition of samples. A laser is focused onto a sample (solid, liquid or gas) to create a plasma. Emissions from the plasma are then collected and analyzed spectroscopically and the atomic spectral lines are used to determine elemental composition. Multivariate analysis is applied to the LIBS data to classify samples based on their compositional differences.

This work is being done to enable measurement by LIBS of samples of materials on the surface of Mars to determine if water is or has been present on Mars.

Materials and Methods

- The ChemCam is an instrument designed to be mounted on the MSL rover mast, and is comprised of a LIBS instrument and a remote micro imager (RMI). A LIBS data base of several carbonate materials is being developed in the laboratory with a system similar to the ChemCam LIBS. Samples include natural rocks collected from various locations, as well as some reference standard samples. The LIBS spectra of calcite (CaCO3), dolomite (CaMg(CO3)2), siderite (FeCO3), and rhodochrosite (MnCO3), have been measured under martian atmospheric conditions (~7 Torr Co2).
- The region of the LIBS spectrum with the most elemental information of the samples was used in the analysis. The multivariate analysis tool of PCA is used which provides a map of samples and variables, helping to identify the variables that relate to the sample and their differences. By using PCA, a new coordinate system is computed (the principal components) which define the variance in the data. The data is reduced as there are typically fewer PCs needed to explain the variance in the data than there are variables in the data set. The PCA scores plot, a projection of samples plotted in the new coordinate system, gives a map of the samples. Similar samples lie closer together than dissimilar samples.
- Analysis was done using The Unscrambler® X ver 10.0.1

Results and discussion

- A PCA analysis of the LIBS Spectra over the range from 460-820 nm was run and samples can be seen to be separated into four groups in the scores plot. From this it can be seen that classification of different carbonate materials is possible based on their LIBS spectra. By adding more samples of the expected classes of materials that may be found on Mars, a model that can identify these materiels will be developed. Likewise regression models can be developed to measure the concentration of major elements in the samples. This will allow for rapid identification of unknown samples during the Mars Rover experiments in 2011.

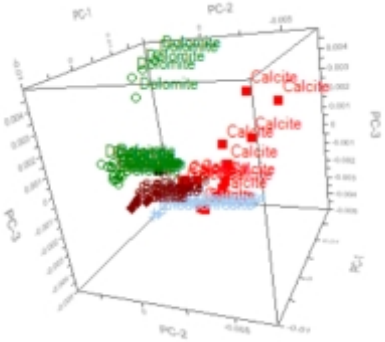

Figure 2: *3-D Scores plot showing separation of the classes of different carbonate materials.*

Application note overview

Software	The Unscrambler® X
Methods	Principal Component Analysis (PCA), SIMCA
Data type	Laser-Induced Breakdown Spectroscopy (LIBS)
Industry	Geology, space exploration
Added Value	During an upcoming exploration of mars, surface rocks will be measured by LIBS with the intent to classify them

Conclusions

LIBS data, with over 6000 variables per sample, are highly multivariate. The use of PCA allows for a rapid visualization of sample groupings and, from this analysis, classification models can be developed to rapidly identify Mars rocks in situ during exploration by the Mars rover.

For complete details of this work please see:

Nina L. Lanza, Roger C. Wiens, Samuel M. Clegg, Ann M. Ollila, Seth D. Humphries, Horton E. Newsom, and James E. Barefield, "Calibrating the ChemCam laser-induced breakdown spectroscopy instrument for carbonate minerals on Mars," Appl. Opt. 49, C211-C217 (2010)