Characterization and comparison of structural and compositional features of planetary quadrilateral pyroxenes by Raman spectroscopy

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ABSTRACT

This study reports the use of Raman spectral features to characterize the structural and compositional characteristics of different types of pyroxene from rocks as might be carried out using a portable field spectrometer or by planetary on-surface exploration. Samples studied include lunar rocks, martian meteorites, and terrestrial rocks. The major structural types of quadrilateral pyroxene can be identified using their Raman spectral pattern and peak positions. Values of Mg/(Mg + Fe + Ca) of pyroxene in the (Mg, Fe, Ca) quadrilateral can be determined within an accuracy of ±0.1. The precision for Ca/(Mg + Fe + Ca) values derived from Raman data is about the same, except that corrections must be made for very low-Ca and very high-Ca samples. Pyroxenes from basalts can be distinguished from those in plutonic equivalents from the distribution of their $Mg^+$ [Mg/(Mg + Fe)] and Wo values, and this can be readily done using point-counting Raman measurements on unprepared rock samples. The correlation of Raman peak positions and spectral pattern provides criteria to distinguish pyroxenes with high proportions of non-quadrilateral components from (Mg, Fe, Ca) quadrilateral pyroxenes.

INTRODUCTION

Laser Raman spectroscopy is well suited for characterization of materials on the surfaces of planets, satellites, and asteroids (Wang et al. 1995). Raman spectroscopy can be used to identify unambiguously most of the rock forming minerals. It can provide additional information on structural and compositional variations for many mineralogical groups, and many rock types can be inferred from sequences of Raman spectra. This technique can also be used to identify reduced carbon down to ~50 ppm in favorable cases (Wdowiak et al. 1997; Wang et al. 2001) as well as other organic species pertinent to the detection of extraterrestrial life on other planets (e.g., Edwards et al. 1999; Wynn-Williams and Edwards 2000). In addition, it is now feasible to build a small Raman system as part of a scientific instrument payload for a rover or lander to carry out planetary on-surface analyses. A breadboard model of such a Raman system has been built in our laboratory (Wang et al. 1998), and a flight Raman system is under development (Haskin et al. 2001). Raman spectroscopy has typically been used in mineralogy to elucidate structure. Use of Raman spectroscopy as a primary tool for identification and characterization of minerals in a routine manner under field conditions is new. It is thus important to determine the accuracy with which Raman spectroscopy can do these tasks, especially on sample surfaces as they are encountered and without special preparation for analysis. In this paper, we show that the pyroxene group of minerals is amenable to such identification and characterization.

The pyroxene group is the most important mineral group in planetary mineral suites in terms of the information recorded about petrogenetic processes (e.g., Papike 1996). Its importance as the major rock-forming silicate on the surface of Mars is indicated by the mineralogy of the shergottite basaltic meteorites (e.g., McSween 1994) and by recent data (the ubiquity of basalt and basaltic andesite) from the Thermal Emission Spectrometer on the Mars Global Surveyor (Christensen et al. 2000). Determining the compositional and structural characteristics of pyroxenes in rocks can be crucial to understanding their petrogenesis. In this paper, we evaluate in particular the feasibility of determining both structure and composition of quadrilateral pyroxene [(Mg,Fe,Ca)$_2$Si$_2$O$_6$] using only Raman spectra as would be obtained from on-surface planetary measurements. Such characterization would also be useful in terrestrial field and laboratory investigations.

Raman spectral features of pyroxene have been extensively studied in the past. Etchepare (1970) reported a study using polarized Raman measurements on a single crystal of diopside. He also made preliminary assignments of 28 observed peaks into Si-O stretch, M-O bond vibrations, and silicate chain deformations. The first Raman spectra of lunar pyroxene were obtained by Fabel et al. (1972) and Perry et al. (1972) on samples returned by the Apollo missions. They reported two strong Raman peaks, one in the 1000–1010 cm$^{-1}$ range and the other in the 650–670 cm$^{-1}$ range. Perry et al. (1972) also sug-