Identification of Modal Abundances in the Spectra of Natural and Laboratory Pyroxene Mixtures: A Key Component for Remote Analysis of Lunar Basalts. Jessica M. Sunshine and Carle M. Pieters, Department of Geological Sciences, Brown University, Providence, RI, 02912.

Reflectance spectroscopy continues to provide new opportunities for remotely assessing the mineralogy of unsampled lunar basalts. Although spectra of basalts contain features that are diagnostic of individual minerals, their spectral features are the combined results of absorption bands from all mineral constituents. As such, the petrologically significant geochemical properties of lunar basalts, their modal mineralogy and the chemical composition of the individual minerals, are difficult to quantitatively extract from their reflectance spectra.

One approach to this problem is to reduce a spectrum into individual absorption bands by modeling it as a sum of mathematical distributions. A model for electronic transition absorption bands was developed by Sunshine et al. [1], that uses modified Gaussian distributions to describe each absorption band in terms of three model parameters; band center, band width and band strength. Sunshine et al. initially used this modified Gaussian model (MGM) to successfully identify absorption bands in orthopyroxene (OPX) and clinopyroxene (CPX) spectra, and to establish compositional trends in absorption bands for a suite of olivine spectra [2].

The MGM can also be applied to spectra of OPX and CPX mixtures. Sunshine et al. previously examined the spectra of a 45-75 µm particle size suite of nine mass fraction mixtures (Figure 1) to determine the variations in absorption band centers as a function of modal abundance. The MGM deconvolution of these pyroxene mixture spectra reveals individual absorption bands that correspond directly to those found in the OPX and CPX endmember spectra. For example, in the spectrum of the 50/50 OPX/CPX mixture (Figure 2), the absorption feature near 1.0 µm is composed of two absorption bands, one from the OPX (large arrow) and one from the CPX (small arrow). The derived band centers for the primary absorptions near both 1.0 and 2.0 µm are at the same wavelengths as the absorptions bands in the OPX and CPX end-member spectra and remain essentially constant throughout the suite of mass fraction mixtures (Figure 3). More recent experiments indicate that band centers are also constant for suites of spectra with <45 µm and 75-125 µm size particles. The band centers are similar for all of the particle size suites, suggesting that measurements of band centers are independent of particle size.

The band strengths of the primary absorption bands in the OPX-CPX mass fraction mixture spectra are also observed to vary systematically with modal abundance. As can be seen in Figure 3, the strength of each of the primary absorption bands changes monotonically with modal abundance. For example, the primary OPX absorption centered at $0.92~\mu m$ (large arrow) becomes increasingly stronger with increasing OPX content in the mass fraction mixtures, while the primary CPX absorption at $1.03~\mu m$ (small arrow) becomes weaker. Similar relationships exist for the primary OPX and CPX absorptions centered near $2.0~\mu m$ ($1.83~and~2.29~\mu m$, respectively). More specifically, the relative ratios of the strengths of the OPX to CPX absorption bands in both the $1.0~\mu m$ and $2.0~\mu m$ OPX regions vary logarithmically as a function of modal abundance (Figure 4). As with band centers, these variations in relative band strength are independent of particle size. In addition, the ratios of the strengths of the OPX to CPX bands are the same for both the $1.0~and~2.0~\mu m$ absorptions.

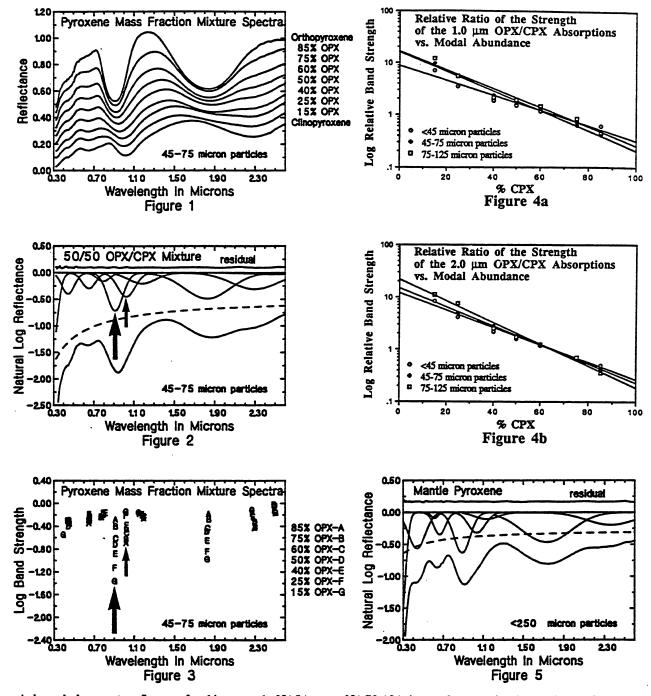
These new relationships observed in OPX-CPX mass fraction mixtures have several implications for modeling unknown spectra. All of the observed systematic variations appear to be largely independent of particle size, indicating that particle size effects on modeling unknown spectra can be considered to be minimal. In addition, the similar ratios of the strengths of the OPX to CPX absorption bands in both the 1.0 and 2.0 μ m regions provides an extra mathematical constraint when modeling an unknown spectrum. This reduces the number of free parameters in the model and would be particularly useful in fitting a spectrum with lower signal to noise. Finally, the logarithmic relationship of band strengths of the 1.0 and 2.0 μ m OPX to CPX absorptions provides a method for estimating the modal abundance of unknown pyroxene mixtures.

A similar approach can be applied to the spectra of natural pyroxene mixtures, such as the mantle sample from Moses Rock Diatreme (Figure 5), which consists of alternating exsolution lamellae of two discrete pyroxenes. The MGM fit to this spectrum shows that the absorption features in the 1.0 and 2.0 µm regions are each composed of two primary absorption bands, one set representing an OPX composition and one a CPX composition. Using the relationships derived from the laboratory mass fraction mixture spectra (Figure 4), the modal abundances of the two pyroxenes can be estimated based on the relative strengths of the OPX and CPX bands. Depending on whether the 1.0 or 2.0 µm data are used, the derived modal abundance for the mantle pyroxene range from 48±3% CPX to 44±2% CPX. This estimated modal abundance is remarkably self-consistent, considering the compositional differences between the two pyroxenes in this natural sample and those used in the laboratory mixtures, and is in excellent agreement with visual estimates.

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The next phase of this research will be to examine spectra of natural samples which exhibit a more continuous zonation in pyroxene composition, as is often found in pyroxenes from lunar basalts [e.g. 3]. Experiments are planned using spectra of CPX separates from the lunar basalt 12063. We would also like to include spectra of synthetically zoned pyroxenes in this analysis, if samples become available. The MGM will continue to be developed and tested on terrestrial, synthetic, and lunar samples as we strive to create a method for remotely extracting petrologic information from spectra of unsampled lunar basalts.

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Acknowledgements: Support for this research, NASA grant NAG9-184, is greatly appreciated. Additional financial support was generously supplied by a Zonta International Foundation Amelia Earhart Fellowship to J. M. S. All spectra used in this study were collected with RELAB, a multi-user facility supported under NASA grant NAGW-748.