

Extraction of Compositional Information from Olivine Reflectance Spectra: A New Capability for Lunar Exploration. Jessica M. Sunshine and Carle M. Pieters, Department of Geological Sciences, Brown University, Providence, RI 02912.

New opportunities to explore the lunar surface using remotely acquired reflectance spectra are expected from the deployment of imaging spectrometers on earth based telescopes, the upcoming Galileo lunar encounters, and the proposed Lunar Observer spacecraft. Although reflectance spectra contain features that are diagnostic of individual minerals, spectra of lunar rocks contain combined absorption features from each of the minerals present on the surface. Mineralogic interpretation of these convolved spectral signals depends on our ability to resolve them into quantifiable parameters that are related to specific minerals. Spectra can be deconvolved by representing the individual absorption bands as discrete mathematical distributions and modeling the spectrum as a sum of these distributions using a least-square fitting procedure. An accurate model for electronic transition absorptions has been developed by Sunshine et al., 1990 (J.G.R. in press) which 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. [1] were able to use this modified Gaussian model (MGM) to successfully resolve the spectra of orthopyroxene, clinopyroxene and pyroxene mixtures into individual absorption bands. The study presented here focuses on applying the MGM to olivine reflectance spectra.

Given the relationship between olivine chemistry and the degree of differentiation of a rock, developing the ability to not only identify the presence of olivine, but also to provide constrains on its chemical composition using remotely obtained reflectance spectra would be particularly useful for lunar petrology. However, the spectrum of olivine is complex (see Figure 1). It is dominated by an absorption feature near 1.0 μm that consists of three overlapping absorption bands caused by the spin-allowed electronic transition of Fe^{+2} in distorted octahedral (M1 and M2) crystal field sites [2,3]. Previous studies using transmission spectra of oriented olivine crystals have revealed systematic compositional trends in the band centers of individual absorption bands [2,4]. Similarly, in reflectance spectra of particulate olivines, the overall minimum (near 1.0 μm) of the composite absorption feature has also been observed to vary with composition [5].

Because the 1.0 μm olivine feature has three independent absorption bands, there are nine free model parameters (a center, strength, and width for each absorption) all within the 1.0 μm region in any model of the olivine spectrum. It is difficult to resolve these overlapping absorption bands in spectra of multi-component lunar rocks, which include absorption features from other minerals. If quantifiable relationships among the model parameters can be determined for olivine spectra, this problem could be greatly simplified, particularly for data with lower signal to noise ratios.

To investigate the relationships among the model parameters, a suite of twelve olivine samples spanning a wide range of compositions was assembled. (We would like to thank R. Burns, E. Cloutis, and the Harvard Mineral Museum for generously providing several of these samples). Bi-directional reflectance spectra from 0.3 to 2.6 μm were obtained for $<45 \mu\text{m}$ particle size separates of these samples using the RELAB spectrometer [6]. One sample (Fo 43) was excluded from further analysis due to its anomalous spectral characteristics; the cause of this behavior is unknown and being investigated further. The remaining samples were all successfully modeled using five modified Gaussian distributions superimposed on a continuum (see Figure 1 for example). Three of the absorptions (bands a, b and c) form the primary Fe^{+2} feature, another consistently occurs on the short wavelength wing of this feature (band d), and the fifth represents the charge transfer absorptions at short wavelengths.

Modeling the suite of olivine spectra reveals that the centers and strengths of absorptions vary systematically with chemistry. Analysis of the resultant model parameters also suggests that each absorption band has a fundamental band width and that three of the four major absorption bands have a similar average band widths in energy. The average band widths and their standard deviations are given in wavelength (nm) and energy (cm^{-1}) in the chart below. Bands a, c, and d have band widths of approximately 3000 cm^{-1} while band d has a width of $\approx 1500 \text{ cm}^{-1}$.

	band a	band b	band c	band d
average band width in nm	228 ± 38	176 ± 8	424 ± 37	115 ± 34
average band width in cm^{-1}	3053 ± 270	1612 ± 24	2870 ± 178	2889 ± 311
approximate band width in energy	3000	1500	3000	3000

Since one would expect the width of an electronic transition absorption to be a function of the crystal field site, the relationships between the average band widths suggest that absorptions a, c and d are from one site and absorption b is from a different site. This is consistent with Burns' assignment of absorption bands a and c to

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transitions of Fe^{+2} in the M1 site and absorption band b to transitions of Fe^{+2} in the M2 site based on transmission studies [2,4]. The origin of the smaller absorption, band d, remains unclear. However, the fact that band d has the same average width as bands a and c suggests that absorption band d also arises due to Fe^{+2} in the M1 site.

The suite of olivine spectra was re-modeled using the MGM with the average band widths for the four absorptions given in the chart above. Constraining the band widths reduces the number of free parameters by four, but has little effect on the RMS residual error of fit. The model fit using average band widths for the Fo 97 spectrum is shown, for example, in Figure 1. It is possible to model all the olivine spectra except the high iron fayalite spectrum (Fo 01) using the average band widths shown in the chart above. In order to fit the fayalite spectrum it is necessary to relax the constraints on the band widths. This suggests that the presence of a large proportion of iron changes the structure of the crystal field site and thus the width of the absorption band. The spectra of high iron olivines (Fo <36) will need to be analyzed more completely in order to determine when this transition occurs.

Constraining the band widths increases the correlation of band centers and band strengths with composition. The relationship between the band centers of the primary absorptions and chemistry are shown as a function of molar percentage forsterite in Figure 2. As was first observed for transmission spectra [4], there is a systematic increase in the wavelength of each of the band centers of the primary absorption bands (bands a, b and c) as the composition becomes increasingly fayalitic. While these band centers are all well correlated to the molar percentage forsterite in the samples, band c has the highest correlation, .975, and spans the largest range of wavelengths.

The high correlation between the band centers of the primary absorption bands in olivine spectra and the chemical composition of the sample suggest that the composition of an unknown olivine sample can be estimated from the position of the band centers derived using the MGM. Recognition of the constant band widths in this analysis of laboratory spectra has reduced the number of free model parameters, which will enhance the accuracy of modelling olivine spectra with lower signal to noise ratios. The results presented here, and in previous study of pyroxene spectra [1], suggest that reflectance spectra can be used to not only identify minerals, but to also estimate their chemical composition by relating their absorption characteristics with those derived from known samples. Expanded studies of the spectral variation of additional minerals over a more complete range of compositions, using terrestrial and returned lunar samples, will provide the capability to obtain compositional information for a larger number of relevant minerals on the lunar surface.

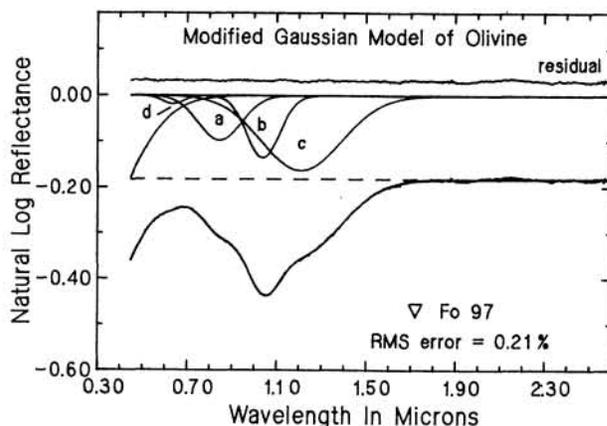


Figure 1. The olivine absorption bands derived from the modified Gaussian model fit to the spectrum of Fo 97 olivine. The band widths used for the primary absorption bands are the average widths indicated in the chart above.

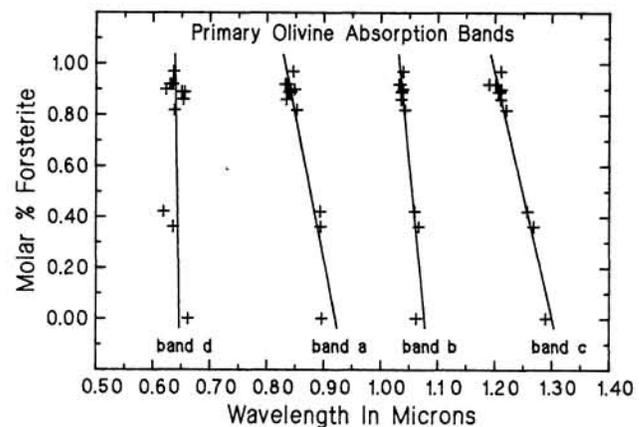


Figure 2. The relationship between band center and composition for the primary absorption bands in olivine reflectance spectra.

References [1] Sunshine, J. M., Pieters, C. M. and Pratt, S. F., *J.G.R.*, 1990 in press. [2] Burns, R. G., *Amer. Min.*, **55**, 1608-1632, 1970. [3] Marfunin, A. S., *Physics of Minerals and Inorganic Materials*, 1979. [4] Burns, R. G., *Mineralogical Applications to Crystal Field Theory*, 1970. [5] King, T. V. V. and W. I. Ridley, *J.G.R.*, **92**, 11,457-11,469, 1987. [6] Pieters, C. M. et al., *RELAB Users Manual*, available on request.