EFFECTS OF GRAIN SIZE ON THE REFLECTANCE SPECTROSCOPY OF OLIVINE IN THE VIS-NIR AND THE DERIVATION OF OLIVINE COMPOSITION USING MODIFIED GAUSSIAN MODELING.

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Introduction: Reflectance spectroscopy has been used to determine mineralogy on planetary surfaces [1-3]. In addition to mineral identification, it is also possible to use reflectance spectroscopy to determine the composition of mafic minerals [4, 5]. Sunshine and Pieters [5] demonstrated that the band center for each of the three bands that make up the broad 1-µm absorption in olivine shifts to longer wavelengths with increasing iron content for fine-grained olivine.

Many confounding factors, in addition to Fo#, may influence an olivine spectrum. There may be compositional zoning within the crystal other transition metals in the M1 and M2 sites, or opaque mineral inclusions. Furthermore, for olivines detected remotely there may be influence from other mafic minerals which are intimately mixed with the olivine. Additionally, Clenet [6] has suggested that increasing grain size may affect the olivine spectrum in a manner similar to increasing iron content. In the present study we attempt to quantify the effects of grain size on the olivine spectrum.

Methods:

Characterization of different olivine compositions and grain sizes. In order to observe the effects of grain size and composition, it was necessary to acquire a suite of olivines with variable iron content. Much effort was put into obtaining a wide range of olivine compositions from forsterite to fayalite. Olivines were obtained from the Caltech Mineral Collection and the Harvard Peabody Museum of Natural History. While many more institutions were contacted regarding olivines of intermediate composition, the availability of these olivines is very low. Intermediate olivine compositions are prone to alteration and substitution of other transition metals in the place of Fe. Additionally, because our study included large grain sizes, it was necessary to obtain ~10 g of olivine from each composition, a large amount for rare samples. Our final olivine suite consisted of four localities: Polar Urals (Fo 90, Ural Moutains, Russia), San Carlos Indian Reservation (Fo 88, Gila, Arizona, USA), Hualalai (Fo 82, Kileau volcano, Hawaii, USA), and St. Peters Dome (Fo 1,Colorado, USA).

The olivines were crushed via sledgehammer at Caltech and other minerals in the rock were removed by careful separation with the aid of a reflected light microscope. Once pure olivine was obtained from each composition, the grains were further crushed using a corundum mortar and pestle and sieved into grain size separates of 0-45 µm, 45-75 µm, 75-125 µm, 125-250 µm, 250-500 µm, 500-1000 µm, and 1000-2000 µm.

The reflectance spectrum from 400-2500 nm of each grain size separate of each olivine composition was acquired using an Analytical Spectral Devices Field Spectrometer at Caltech. In order to obtain these measurements the spectrometer was calibrated using a Spectralon 99% reflectance standard The samples were then measured over surfaces with nearly constant and low albedos to mitigate any background influence.

The three high Fo# olivine samples were then measured using an electron microprobe in order to quantify the amount of trace elements and other phases which may be present. Large grains were selected from each olivine in order to see any effects due to zoning of olivine.

Modified Gaussian Modeling Program. Sunshine has suggested that the standard gaussian equation, which as been used in the past [7], is not appropriate for modeling electronic transitions because the shape of these absorptions is dominated by randomness with regard to band length and not energy of absorption [4]. Therefore, a modified gaussian has been developed which more accurately represents the electronic transitions [4]. A software package for determining the best fit of modified gaussian parameters for deconvolution of a given spectrum, the Modified Gaussian Modeling program (MGM), has been developed by Sunshine. This software is available to the public [8]. Using this software and a suite of olivines ranging in composition from Fo 97 to Fo 01, Sunshine has reported trends between composition and band center, strength, and width in the three individual absorptions which make up the 1-µm feature [5]. The software along with these trends have been used to estimate the composition of olivine remotely (e.g. [2, 9, 10]).

Use of the MGM program requires an initial estimate by the user for the gaussian parameters (center, strength, and width) which make up the absorption features. Change in input parameters can therefore result in differing outcomes. To overcome the subjectiveness necessary for initial estimates, we replicate the procedure used by Clenet for automated calculation of these input parameters based on width and strength of the broad 1-µ feature [6].

We have deconvolved all of our acquired olivine spectra using the techniques of Clenet and Sunshine, mentioned above. We have compared variations in the olivine parameters with both grain size and composition.

Results: Our electron microprobe analysis showed that other transition metals are minor constituents in our olivines. We did not observe any significant change in composition with proximity to the grain cores. This implies our sample set is well-suited to test, changes based on changes in Fo# and grain size alone, absent confounding factors.

Grain size has a widening effect on the broad 1-µm absorption feature of olivine. There is also a consistent darkening of the spectrum with increasing grain size (Fig. 1). The widening observed with increasing grain size is, to a first order, similar to the widening observed with increasing iron content. The deconvolution of our olivine spectra indicate that for grain sizes larger than 125-µm, the positions, of the absorptions, which are most indicative of composition, no longer correspond with the compositional trends found by Sunshine. This result confirms earlier work done by Clenet [6]. Examination of strengths and widths show significant deviation as well. In particular, values for strength and width which lie far outside of the narrow parameter range given by Sunshine for the olivine suite have been produced by the MGM program (Fig. 2). Strikingly, the program has returned these extreme values for both large and small grain sizes.

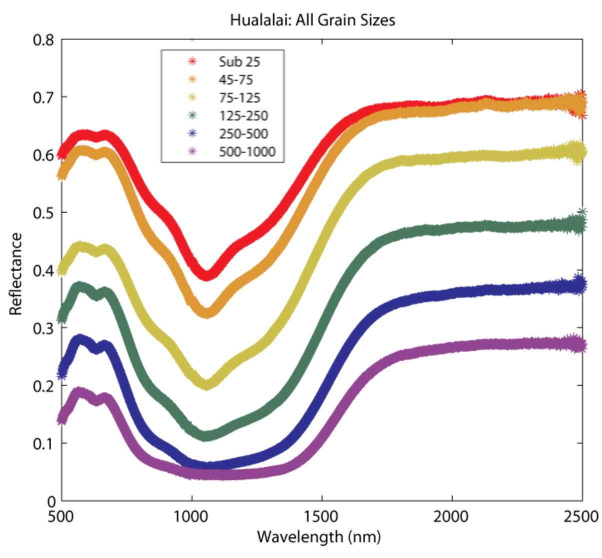

Figure 1 (Above): Reflectance spectra of Hualalai olivine (Fo 82) for various grain sizes. Note the widening, flattening, and darkening of the spectra from sub 25-µm to 500-1000-µm

Conclusions: The current version of the MGM program is capable of returning parameter values which lie far outside of the bounds set by previous work. This may be because of the effects of Fo#; however, the lack of boundary conditions may contribute. Additionally, it is possible that the need for an initial estimate of parameter values also causes the program to fall into a local minimum of error because not all combinations of parameters are explored.

Future Work: A new version of the MGM program is being developed which removes the need for an initial estimate. This program, rather than utilize current techniques for finding a best fit, is brute force in that all possible parameter combinations are explored. The possible parameter values are also limited to bounds set by previous work. We will test our high Fo# samples again with this approach.

Intermediate olivine compositions (Fo# 10-70) are still being sought. Analysis of these intermediate olivines may further elucidate any trends in grain size and compositional effects.

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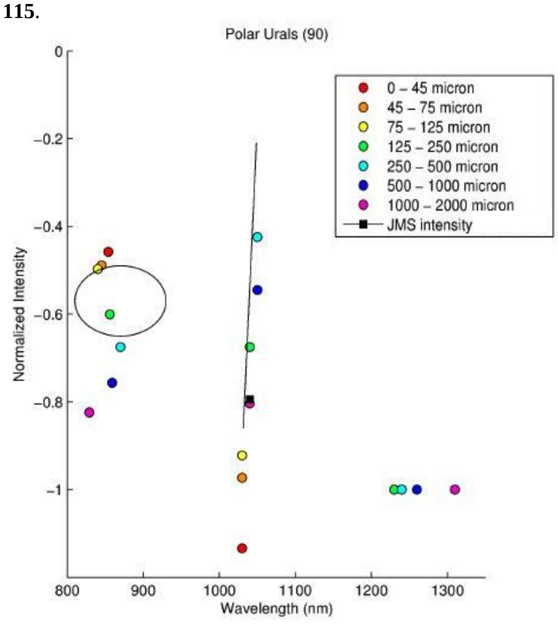

Figure 2 (Right): Intensity of the three bands which make up the broad 1-µm feature of olivine. The intensities are normalized by the strength of the third band. Black circle/line indicate the range in strengths found by Sunshine for the first and second absorptions for all olivine compositions. Note that even small grain sizes fall outside these ranges