

Lucey et al.: Spectral survey of small lunar craters, American Mineralogist NovDec 2014, Supplement

Appendix

We use a mineral abundance extraction algorithm similar to that used by Cahill and Lucey (2007). Spectrum libraries are computed for the system plagioclase, low-Ca pyroxene, high-Ca pyroxene, olivine, and nanophase iron of two sizes with different optical effects. The foundation of the compositions are the ternary system of olivine and the two pyroxenes computed at 10% intervals for a total of 66 compositions. These compositions are then mixed with plagioclase at 1% intervals from 0–100% plagioclase for a total of 6600 compositions. These compositions in turn are mixed with seven amounts of nanophase iron to simulate space weathering effects. Nanophase iron includes optically small material modeled by (“submicroscopic iron”) Hapke (2001) and studied by Noble et al. (2007) and Noble and Lucey (2007), and larger nanophase iron that we call Britt-Pieters particles (Lucey and Riner 2011; Britt and Pieters 1994) that are an important darkening phase in lunar soils. The abundances of these two components are matched to the measured abundances of these phases in the LSCC soils. For simplicity the abundance of the two sizes are linked by the relationship Britt-Pieters (wt%) = 2* submicroscopic iron (wt%) that causes the libraries to occupy the same spectral space as the LSCC data in terms of reflectance and continuum slope. We remove a continuum from all of the model spectra (6600×7) and from the unknown spectrum (for example, one of the LSCC spectra) and we find the closest spectral match and use the composition associated with that model as the mineral composition of that spectrum.

The comparison between the libraries and the spectrum under analysis is an evenly weighted average of the correlation of the library and target spectra after removal of a continuum, and the sum of the absolute value of the total of the difference between the library and target spectra. The correlation metric emphasizes the similarity in the shape of the spectrum, while the difference metric includes band intensity as an important parameter.

We plot the result of exercising the mineral mapping algorithm in Figure A1 showing there is a poor correlation of the model and measured mineralogy (>20 wt% error). However, the behavior of the model against individual minerals provides clues to its shortcomings. The low correlation is due to systematic over and under-prediction of specific minerals, for example, olivine is greatly overestimated. Furthermore, we find that forward modeling of the LSCC compositions (using the LSCC compositions as inputs to compute a reflectance spectrum) produces a set of spectra that do not match the observed trend of band minimum vs. the ratio of low-Ca to total pyroxene (Fig. A2).

Successful estimates of relative abundance of minerals in an assemblage using a mixing model requires at the minimum that the relative intensities of the bands of the end-members accurately reflect the relative intensities of the bands in the unknown spectra. An error in the relative intensities will give rise to an error in estimated abundance. For example, if an end-member intensity is strong relative to the intensity of that component in the mixture undergoing analysis, then the abundance of that component will be underestimated because a lower abundance is adequate to match the band strength of the target spectrum than is actually present. While significant attention has been paid to determining the optical constants of the rock forming minerals within the major mineral classes, especially olivine and pyroxene (Trang et al. 2013; Denevi et al. 2006) little work has been done to calibrate between classes of minerals. Furthermore, even within mineral classes there are large discrepancies between optical constant intensities derived from sample sets prepared by different investigators. The best documented case was presented by Trang et al. (2013) who showed that there is a factor of four discrepancy between the derived band intensities using the data of King and Ridley (1987) vs. the data of Sunshine and Pieters (1998). Interestingly, Sunshine and Pieters (1998) analyzed both of these data sets using MGM, and found they were completely consistent with respect to the absorption band parameters width and center, and even the relative intensities of the olivine bands. However, Trang et al. (2013) showed that the King and Ridley (1987) data are systematically lower in albedo, and exhibit systematically stronger absorption bands than the data presented by Sunshine and Pieters (1998). Because the optical constants are derived from reflectance spectra using a model that does not include the unknown cause of this difference, the

estimated optical constants also contain the corresponding uncertainty in intensity. While the existing optical constants are a starting point in understanding the composition of an unknown spectrum, with testing and validation data the accuracy can be improved by pinning the relative intensities of the end-members to ground truth. The data set of the LSCC is that ground truth for lunar spectral studies.

In addition to intensities, the radiative transfer model should also obey observed spectral trends in the validation data set. We find that forward modeling of the LSCC compositions using (using the LSCC compositions as inputs to compute a reflectance spectrum) produces a set of spectra that do not match the observed trend of band minimum vs. the ratio of low Ca to total pyroxene (Fig. A2) indicating that the low-Ca pyroxene end-member exhibits a band center that is too long in wavelength, and the high-Ca pyroxene end-member exhibits a band center that is too short in wavelength.

For these reasons, to improve the estimation of abundance as characterized by the performance of the algorithm against the LSCC data, we elected to treat the band intensities of the four minerals as free parameters in an optimization. To ameliorate the trend problem shown in Figure A2, we also allowed the pyroxene optical constants to “float” in wavelength. We performed a high-fidelity grid search of space defined by the 6 parameters adjusted. We found the best performance with a shift of the low Ca-pyroxene imaginary index spectrum of Lucey (1998) (computed at an Mg-number of 65) by 12.5 nm to shorter wavelengths, and the high-Ca pyroxene imaginary index spectrum by 50 nm to longer wavelengths, in increase in intensity of the olivine imaginary index spectrum by a factor of seven, and that of plagioclase by a factor of two gave rise to this improvement. The intensities of the imaginary index spectra of the two pyroxenes remained unchanged.

A factor of seven in intensity increase in the olivine intensity (relative to pyroxene) may seem extremely large, however, note Trang et al. (2013) documented a factor of four difference in absorption intensity within reported olivine spectra. Furthermore, the olivine was computed at an Mg-number of 65, while the LSCC average olivine composition is somewhat less magnesian. Finally, the fits may be compensating for a systematic difference between the olivine and pyroxene in ways not accounted for in the model, for example surface texture or internal scattering that can affect the reflectance spectrum.

The result of this optimization was a significant improvement in performance as shown in Figure 8 (main text). The mean error in mineral estimation is 8%, down from the 25% using the original values. Olivine and high-Ca pyroxene are no longer grossly overestimated, and plagioclase shows better correlation. Turning back to the trend of band minimum vs. low-Ca pyroxene over total pyroxene, forward modeled spectra of the LSCC compositions are much more consistent with the LSCC data than the previous effort (though not exact) (Fig. A3). The ability of the model to retrieve the LSCC abundances with <10% error is similar to the formal error in extraction of Mars compositions from TES data (Hamilton and Christensen 2000).





