A large spectral survey of small lunar craters: Implications for the composition of the lunar mantle

Paul G. Lucey¹, Jessica A. Norman¹, Sarah T. Crites¹,², G. Jeffrey Taylor¹, B. Ray Hawke¹, Myriam Lemelin¹,²

¹Hawaii Institute of Geophysics and Planetology, University of Hawaii at Manoa, 1680 East West Road, Honolulu HI 96822, USA
²Department of Geology and Geophysics, University of Hawaii at Manoa, 1680 East West Road, Honolulu HI 96822, USA

Abstract

A global spectral survey of 4506 immature craters with diameters less than 1 km was carried out using near-IR data from the Kaguya Spectral Profiler in order to characterize the composition of the lunar megaregolith. On the basis of band minima and radiative transfer mixing models, small crater spectra fall into three groups: 1) mare basalts with strong absorptions at relatively long wavelengths indicating high ratios of high to low Ca pyroxene; 2) norites containing about 50% plagioclase and with pyroxene assemblages dominated by low-Ca pyroxene that occur within the South Pole-Aitken Basin (SPA), near Apollo 14 and other locations near Imbrium Basin, and three major cryptomaria deposits;
and 3) noritic anorthosites occurring within the Feldspathic Highlands Terrane containing about 20 wt% pyroxene with a pyroxene assemblage containing exclusively very low Ca pyroxene. Very few pure anorthosites are present in this survey and there are no occurrences of pyroxene-poor olivine-rich assemblages. Models of the composition of basin ejecta incorporate large amounts of mantle material and the spectral results require that the sampled mantle is orthopyroxenite. Basin depth-diameter ratios used in the models required to match the measured composition are consistent with prior estimates for the largest basins. The composition found in the SPA and Imbrium regions are consistent with mafic impact melt breccias or basaltic impact melts of basin origin. For SPA we model this composition and find it requires an extremely low impact angle. While this is consistent with prior work on an oblique impact for the SPA event, a more robust solution invokes the production of norite in impact melt seas.

Introduction

One of the more intriguing observations in lunar remote sensing was made by Pieters 1986 who noted a significant difference between the noritic composition of the uppermost crust inferred from spectra of small craters, and diverse mineral assemblages observed in central peaks. Pieters indicated that it seemed not possible to arrive at the noritic composition by mixing the observed deeper compositions and proposed a number of hypotheses to account for the observations. These included compositional gradients imposed on the crust during magma ocean crystallization, post-magma ocean igneous intrusions into the crust, or deposition on the surface of material deeply excavated by major impact basins.
In Pieters 1986 the small crater sample comprised craters 5 km or smaller, based principally on the spatial resolution limitations of the groundbased spectroscopic technique then available. With the abundant new spectral data now available we can expand the sample of small craters to all longitudes, and include smaller craters. Pieters acknowledged that her inclusions were based on a relatively small sample; expanding that sample is the goal of this paper.

We present the results of spectral analysis of about 2700 lunar highland craters occurring at latitudes within 50 degrees of the equator and at all longitudes. We analyze these data with an empirical comparison of the spectra of the craters with the well-documented spectral and compositional data of the Lunar Soils Characterization Consortium (LSCC) data (Taylor et al, 2001, 2010) and with radiative transfer mixing models. We place these results into context using models of basin excavation and basin melt formation to test the hypothesis that the materials of this crater population represent basin ejecta, or basin impact melt.

Data

Visible and near-infrared spectra from the Japanese Space Agency (JAXA) SELENE (Kaguya) Spectral Profiler (SP) were used for the survey. SP obtained a global sample of spectra of the lunar surface at a resolution of ~550 m from 0.5 to 2.4 µm in the form of single pixel, largely nadir profiles along the track of the polar orbit of the SELENE satellite (Haruyama
et al. 2008; Matsunaga et al. 2008; Yamamoto et al. 2010). During the course of the SELENE mission the orientation of the plane of the satellite orbit with respect to the Moon-sun line--the beta angle--varied widely so optimal lighting conditions where the solar incidence angle is at a minimum occur only in portions of the data (the illumination history of the SP experiment is given in Yokota et al. 2011). Numbered by orbit (“revolution” in JAXA’s terminology), revolutions between 4000 and 5000 were particularly well-illuminated so this survey used that range of data. Of the 1000 orbits in this range, 467 were used for the survey comprising approximately five million spectra. The data were photometrically corrected using the equations of Yokota et al. 2011 using the “highland” photometric parameters.

To detect the desired craters for this survey, the first criterion was to cull out mature locations from the data. The space weathering parameter OMAT (Lucey et al 2000) was computed from the data using the constants provided in that paper, and a cutoff of 0.25 was applied to the data to isolate candidate immature locations. OMAT includes apparent reflectance as an input parameter and so is sensitive to variations in that quantity due to topographic shading. To minimize that effect and also to maximize signal-to-noise ratio, analysis was also confined to latitudes within 50 degrees of the equator. This culling resulted in a total of 37,870 candidate spectra with high OMAT values indicating likely immature locations. Because mass wasting and large recent craters can produce fresh surfaces not associated with small craters, and the remaining topographic shading can cause OMAT artifacts on sun-facing slopes, each candidate location was visually inspected using Kaguya Multiband Imager (MI) data and classified as a small crater, large crater or
other geologic feature. This resulted in identification of 4506 individual immature craters less than 1 km in diameter. For the many of these craters more than one SP spectrum occurs within one crater radius from the rim so the entire data set comprises 8184 individual spectral measurements. The global distribution of these small crater samples is shown in Figure 1. Along with OMAT we also computed FeO using the equations of Lawrence et al. 2000. Using FeO as a way to discriminate mare craters from highland craters, the data contain about 2700 non-mare craters on the basis of FeO contents less than 12 wt.%. Analysis Two methods are applied to analyze these data: estimation of the average pyroxene chemistry, and deriving modal abundance of the major minerals. We estimate pyroxene chemistry by deriving the minimum position of the 1-µm band due to iron in mafic silicates and comparing this to data from the Lunar Soils Characterization Consortium (LSCC). In most lunar soils the 1-µm band minimum is related to the pyroxene chemistry because of the dominance of lunar soils spectra by pyroxene. While the band position is affected to some degree by iron content, the largest effect is due to the average calcium content (Adams 1974; Hazen et al. 1978; Cloutis 1985; Klima et al. 2007, 2011; Denevi et al. 2007). In the complex mixture that is lunar soils, the average pyroxene chemistry can be expressed as the ratio of low Ca pyroxene to total pyroxene as lunar soils typically contain more than one pyroxene. The LSCC data show a clear correlation of low Ca pyroxene to
total pyroxene with band minimum, and we will quantify and use this relationship to interpret the small crater database.

The position of the minimum in this study is determined first by removing a straight-line continuum by division from each spectrum by defining a line from reflectance values at the wavelengths of 0.75 and 1.5 µm. We then locate the minimum spectral channel between the continuum wavelengths, and finally fit the continuum-removed spectrum with a 2nd order polynomial within fifty nanometers of the minimum spectral channel. We report the minimum value of that polynomial as the band minimum. The fitting processing mitigates the quantization that would occur if only the minimum spectral channel were taken as the actual minimum. In a minority of cases a portion of the spectrum near 1.1 µm exceeds unity in spectra with the continuum as defined removed; in these cases a three point continuum is defined using a parabola as the continuum function and the minimum derived as above in the 1-µm region.

To directly connect the band minima of the small craters to those of to lunar samples, we compare these results to the band minima of a portion of the Lunar Soils Characterization Consortium (LSCC) data. These data comprise 19 soils spanning the full range of composition present at the Apollo landing sites. These samples were sieved into several size fractions; we use the 10-20 µm size fraction as this fraction was found to be most similar to the spectra of the bulk soil (Pieters et al. 1993). In the LSCC data set, pyroxenes are classified into four types: high and low iron clinopyroxene, pigeonite (low Ca clinopyroxene) and orthopyroxene. For this study we classify pigeonite and orthopyroxene
as “low Ca pyroxene” and the two more calcic pyroxene types as “high Ca pyroxene.” We
note here that we will be using the term "norite" for rocks containing pyroxene
assemblages dominated by with low-Ca pyroxene chemistries and gabbro for rocks
containing high-Ca pyroxene chemistries. However, a pigeonite-dominated rock would be
technically a gabbro, but spectroscopically, pigeonites resemble orthopyroxenes more than
they do clinopyroxenes, even though pigeonites are, structurally, more often monoclinic.
We should also note that as will be shown below many of the craters analyzed exhibit band
minima too short to contain significant pigeonite.

As expected, the data from LSCC shows a correlation between the band minimum and the
relative abundance of low and high Ca pyroxene (Figure 2, r=0.88) that we use to construct
a calibration equation. A simple regression between these quantities to produce a
predictive equation gives rise to unrealistically short long wavelengths for mixtures
dominated by low Ca pyroxene (that is, band minima near 0.9 µm), undoubtedly due to the
relatively small sample size and range of the parameter in these data. To arrive at a
calibration consistent with prior measurements of the spectral properties of pyroxene, we
fixed the band position of pure low Ca pyroxene at 0.905 µm corresponding to the shortest
wavelength observed in that mineral (Klima et al. 2007, 2011), and fit the LSCC data forced
through that data point. With this constraint, the predictive equation for pyroxene
composition is:

\[
\text{Low Ca Pyroxene/Total Pyroxene} = 6.7 \times (\text{band minimum} - 0.905)
\]
Applying this equation to the LSCC data, the uncertainty in prediction of low-Ca pyroxene / total pyroxene is 0.085 on a scale of 0 to 1. This equation will form the basis for the interpretation of the small crater band minima.

Figure 3 shows the histogram of band minima for the small crater data set, showing a distinct bimodal distribution representing the difference in pyroxene composition between mare and highland. Mare craters contain high-Ca pyroxene as indicated by the mode near 0.97 µm, and highland craters contain more low-Ca pyroxene as indicated by the mode near 0.91 µm. To investigate spatial variations in this parameter, we interpolated the data to a gridded product at 1 degree resolution shown in Figure 4. The mare-highland dichotomy in average pyroxene chemistry is evident, but there are also strong variations outside the maria, with the largest distinction being the difference between the interior of the South Pole-Aitken basin (SPA) and the more feldspathic highlands. This gridded product includes averaging; in Figure 5 we present histograms of the band minima histograms of spectra occurring within SPA and the Feldspathic Highland Terrane north of SPA as defined by Jolliff et al. 2000. The two terranes differ distinctly in the position of their band minima, with the FHT having a mean band minimum wavelength of 0.906 +/- .008 and SPA showing a mean of 0.922 +/- .010. To further understand the distribution of these distinct units on the basis on their minima, (Figure 6) shows the locations of spectra with band minima within one sigma of the mean of those of the interior of SPA and the FHT. Spectra with SPA-like minima occur in the vicinity of Imbrium and a significant cluster near the Apollo 14 site. Clusters also appear at the major cryptomaria of Schiller-Schickard, Balmer-Kapteyn and Lomonosov-Fleming. Spectra with minima close to those in the FHT
are somewhat more uniformly distributed, but almost absent in the Imbrium region and
within SPA. There is little geographic overlap in the distributions of the two spectral types.

The average spectra of the small craters in these terranes are typical of relatively fresh
feldspathic and mafic highland material (Figure 7). The FHT spectra show weak 1-µm
bands with about 5% deep mafic bands, and a strong shoulder near 1.25 µm due to
feldspar. These correspond to the spectral type N-1 of Pieters 1986 that she interpreted to
be “...feldspathic, minor low-Ca pyroxene (orthopyroxene) component...” The SPA spectra
have about twice the band depth indicating a higher abundance of mafic minerals, and also
exhibit a shoulder at 1.25 µm due to feldspar, and correspond to spectral type N-3 of
Pieters 1986. This type was interpreted to be: “...noritic composition; minor Ca pyroxene ...”

Using the LSCC-derived calibration, the low Ca pyroxene / total pyroxene ratio of the small
crater population of the FHT is 0.99 +/- .05, whereas the small craters within SPA and
regions with similar spectra have a value of 0.88 +/- .07. The implications of these results
are discussed below.

While the pyroxene chemistry is of high interest, the abundance of the major minerals is
also important and we derive these using radiative transfer modeling. Our analysis is
based on the work of Hapke (1981, 1993, 2001) and versions of our implementation has
been presented in Lucey, 1998; Clark et al. 2001; Lawrence and Lucey 2007; Denevi et al.
2008; Cahill et al. 2010. For this study we developed an improved mineral abundance
algorithm that returns mineral abundances with under 10 % accuracy (Figure 7). The
Supplement/Appendix describes the algorithm used and the basis for its improvement.
Using the improved algorithm, we find significant differences in the estimated mineralogy between craters of the FHT and those of SPA. Like the empirical band minimum analysis, we find that the FHT spectra show higher abundances of low-Ca pyroxene than found in spectra occurring within SPA (and similar spectra), and in fact the models return almost no high Ca pyroxene in the FHT and a few percent within SPA.

Mineralogical anomalies are very rare. In the entire small crater database of 8184 spectra, only 13 have band minima near 1.25 µm indicating the presence of pure anorthosite (that is exhibit weak or absent pyroxene bands) and all but three of these are very near the rings of Crisium. There are no analogies to the central peaks of Copernicus (Pieters 1982) or the olivine-rich locations identified by Yamamoto et al. 2010 where pyroxene is a minor component.

Discussion

The extensive sampling here underscores and strengthens the observations made by Pieters (1986). The spectral character of the small crater population of the FHT, away from SPA, Imbrium and cryptomaria is exclusively noritic in the strict sense, with no evidence for significant high Ca pyroxene. The absorption band minima exhibited by these spectra are uniformly at very short wavelengths (Figure 5) indicating that this material contains only orthopyroxene as a mafic phase.
The FHT composition can be modeled as mechanical mixing and emplacement of ejecta composed of pure anorthosite crust with an underlying orthopyroxenite mantle. Following the method detailed in Crites et al. (this volume) we model the crustal composition of the FHT as the average of the ejecta of the 43 largest lunar basins identified by Spudis (1993), including SPA. The ejecta composition of each basin was modeled based on the volume percent of mantle and crust excavated following the basin ejecta volume calculations of Spudis (1993). In this approach, the final composition is controlled by the diameter of the basin, the depth/diameter ratio, and the crustal thickness. The ejected volume is treated as a spherical cavity intersecting a spherical moon. The circle defined by the intersecting spheres is taken as the basin transient cavity and its diameter is fixed at the transient cavity diameter estimated for each basin by Petro and Pieters (2004). The depth associated with the depth-diameter ratio is defined as the distance between the deepest point on the excavation cavity sphere and the surface of the lunar sphere directly above this point. The depth-diameter ratio of the excavation cavity is the excavation depth divided by the diameter of the circle representing the transient cavity. This ratio can be varied arbitrarily by adjusting the distance of the excavating sphere from the center of the Moon and the excavating sphere’s radius. The Moon is modeled as a shell of pure orthopyroxenite mantle, overlain by a shell of anorthosite, in this case 2% orthopyroxene and 98% plagioclase. Varying depth diameter ratio and crustal thickness allows us to arrive at an average basin ejecta composition matching that of the FHT. Two crustal thicknesses were used, 34 and 43 km from the average crustal thickness estimates of Wieczorek et al. (2013), and these gave rise to basin depth diameter ratios of 0.059 and 0.074 to match the observed composition of the FHT. For context, a wide range of
theoretical methods, experiments, and observations agree that for craters ranging in size
from centimeters to tens of kilometers, the depth to diameter ratio for the Moon is
However, modeled excavation cavities based on gravity data by Wieczorek and Phillips
(1999) for the three largest lunar basins (Serenitatis, Imbrium, and SPA) fall off this trend,
with the depth:diameter ratios for Serenitatis and Imbrium estimated near 0.05, and for
SPA 0.01 or even shallower. Although in our calculations we modify the depth:diameter
ratio for all 43 basins, approximately 70% of the total ejecta and over 90% of the mantle
material is derived from the 3 largest basins so our results are dominated by these basins,
and our relatively shallow depth:diameter ratios are in agreement with the observations of
Wieczorek and Phillips (1999). Notably, for a maximum crustal thickness of 60 km
observed in the center of the FHT by Wieczorek et al. (2013), a depth:diameter ratio of
almost exactly 1:10 produces the FHT composition from an orthopyroxenite mantle and
anorthosite crust.

Turning to the spectral type exposed at SPA and elsewhere, the interior of the basin likely
exposes abundant impact melt from its formation (e.g. Petro and Pieters, 2004). Based on
that assumption, we investigated the ability to arrive at the SPA composition using the
same two layer model used above, but this time modeling bulk melt composition. We
assume the melt is derived from a spherical volume tangent to the lunar surface that will
include proportions of crust and mantle depending on the crustal thickness and the sphere
diameter following the method of Vaughan et al. (2013). We calculated the total melt
volume for SPA using the scaling relationship derived by Abramov et al. (2012) and the
model inputs of Kring et al. (2012) and used that to calculate the size of the melt sphere. We calculated the fraction of crust and mantle material in the melt based on this simple geometry and derived the bulk melt composition based on our two-layer model. We varied the crustal thickness and the angle of the SPA-forming impact and found a narrow range of parameters that could produce the observed SPA norite composition assuming a pure plagioclase crust and an orthopyroxenite mantle. The statistically most likely impact angle of 45 degrees (Melosh 1989) requires an unreasonably thick anorthositic crust of 140 km to match the SPA small crater composition. A highly oblique impact angle of less than 6 degrees is required for our calculations to permit a crustal thickness at or below 60 km, the maximum crustal thickness observed by Wieczorek et al. (2013). This conclusion is consistent with prior work concluding that SPA was likely an oblique impact (e.g. Schultz 1997, Garrick-Bethel and Zuber 2009).

Implications

The problem posed by Pieters (1986) was that the composition of the materials excavated by central peaks, presumably representing a large section of the crust, is not similar to the noritic composition revealed by the small crater population. The work reported here reinforces that problem by showing the apparent compositional difference between the two populations (central peaks of large craters and deposits of small craters) is not an artifact of poor sampling of the small crater population. This apparent conflict is resolved by recognizing that mantle must comprise a large fraction of basin ejecta (as shown by previous work and modeling done above), and that its ultramafic composition will cause it
to dominate the mafic composition of a mixture of anorthositic crust and ultramafic mantle.

The extreme noritic nature of the small crater population requires that montle composition incorporated into basin ejecta must be largely orthopyroxenite.

This simple two-layer model ignores a crust that may become more mafic with depth. This has been widely hypothesized and assumed (e.g. Ryder and Wood, 1977), and if true would reduce the amount of mantle required in models to account for the observed total mafic content, but also reduce the basin depth:diameter ratios needed to account for the observations to values below all prior estimates (see calculations in Crites et al. this volume that explicitly deal with this case). The extreme noritic composition observed requires that any more mafic lower crust shares the same relatively extreme low-Ca pyroxene mineralogy as the mantle, as there is no evidence for additional mafic components in the small crater data.

The spectral type exposed at SPA and the Imbrium region likely represents a basaltic impact melt generated by these large impacts. The melts generated by the SPA and the Imbrium impact events were formed from total melting of a large column that extended into the mantle, a composition that explains the mafic nature of these deposits. However, recently Vaughan et al. (2013) have emphasized and demonstrated the potential importance of differentiation of impact melt pools in large basins, and showed that the upper norite layer seen in some impact melt differentiation models is consistent with observations at SPA. The spectral data here are consistent both with a quenched impact melt formed of an orthopyroxenite mantle and an anorthosite crust, and also with
differentiation of an impact melt sea, provided the norite layer is thick enough and close
enough to the surface to dominate the surface composition. Even in the presence of other
styles of differentiation, a quenched crust may be expected atop melt seas, and preserved in
this small crater population. The slightly higher Ca content implied by the difference in
band minimum position observed between the FHT-like spectra and SPA-like spectra is
consistent with a melt formed from orthopyroxene and plagioclase providing a more calcic
melt relative to the very low calcium mantle orthopyroxene source that enabled
crystallization of a somewhat higher Ca pyroxene than the source. We favor the Vaughn et
al. (2013) model of a differentiated melt sheet owing to the need for a quite extreme impact
angle to achieve the proper composition without differentiation.

Finally, we note that the common occurrence of SPA-like spectra within major cryptomaria
suggest they are unlike more recent mare basalts in pyroxene chemistry as pointed out by
Hawke et al. 2005, with our new finding being that their pyroxene assemblage is much less
calcic that typical mare basalts. We take the spectral similarity of the cryptomaria to the
small craters within SPA to be a coincidence, however, it should be considered that the
deposits of these craters may not indicate the presence of unusual mare basalts, but rather
are excavated mafic melt sheets.

References


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<table>
<thead>
<tr>
<th>Rock Type (Stoffler et al. 1980)</th>
<th>FHT</th>
<th>SPA</th>
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<tr>
<td>Noritic Anorthosite</td>
<td>80.4% +/- 5</td>
<td>56.4% +/- 17</td>
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<tr>
<td>Pyroxene</td>
<td>19.6% +/- 5</td>
<td>41.6% +/- 14</td>
</tr>
<tr>
<td>Olivine</td>
<td>0.03%* +/- 1</td>
<td>1.9%* +/- 3</td>
</tr>
<tr>
<td>Low Ca Pyroxene/Total</td>
<td>0.99 +/- .01</td>
<td>0.95 +/- .07</td>
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We use a mineral abundance extraction algorithm similar to that used by Cahill et al. 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 (2008), 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 (6600x7) 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 (greater than 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 (Figure 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 endmembers 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 endmember 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. 2012; 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. 2012 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. 2012 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 endmembers 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 (Figure A2) indicating that the low-Ca pyroxene endmember exhibits a band center that is too long in wavelength, and the high-Ca pyroxene endmember exhibits a band center that is too short in wavelength.

For these reasons, in order 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 2012 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 an 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) (Figure A3). The ability of the model to retrieve the LSCC abundances
with less than 10% error is similar to the formal error in extraction of Mars compositions
from TES data (Hamilton and Christensen, 2000).
Figure 1. Locations of all craters used in this survey. Background image is Kaguya topography. The greater density of points in the maria reflect the presence of thin regolith permitting the small impacts studied in this work to create abundant fresh material from competent underlying material.
Figure 2. Band minimum vs. ratio of low Ca pyroxene for 19 soils of Taylor et al. 2001, 2010 (squares). The solid line is the linear regression to these data. The dashed line is the fit forced through a value of 0.905 for pure low Ca pyroxene.
Figure 3. Histogram of band minimum for the small survey crater data set. The peak near 0.97 microns corresponds to the lunar maria, and the peak near 0.9 microns corresponds to the lunar highlands.
Figure 4. Map of band minimum. Data ranges from 0.9 (black) to 0.97 (white). The long wavelengths exhibited in the maria indicate dominance by high Ca pyroxene. Outside the maria two units are apparent, very short values corresponding to the Feldspathic Highland Terrane (blue tones) and slightly longer wavelengths occurring within South Pole-Aitken Basin and some cryptomaria.
Figure 5. Histogram of band minimum for the Feldspathic Highlands Terrane (red) and South Pole-Aitken Basin (black) illustrating the offset in band minimum, and hence composition. A few small mare exposures occur within both units as seen in the “long tail” of the distribution.
Figure 6. Locations of spectral types based on band minimum. Red diamonds: maria; green dots, spectra with band minima similar to those in South Pole-Aitken Basin; blue dots, spectra with band minima similar to those in the Feldspathic Highlands Terrane.
Figure 7. Average spectra of SP-A small craters (black) and FHT small craters (red).
Figure 8. Correlation of measured and modeled LSCC soil mineralogy using the algorithm described employing the algorithm described in the Appendix. Mineral abundance prediction is about with ~ 8 vol % error in predicted mineralogy. Green: olivine; red, high Ca pyroxene; blue, low Ca pyroxene; black circles, feldspar.
Figure A1. Correlation of measured and modeled LSCC soil mineralogy using the algorithm described. Green: olivine; red, high Ca pyroxene; blue, low Ca pyroxene; black circles, feldspar.
Figure A2. Black squares are the LSCC soils with a regression fit to the data. The diamonds are the locations of spectra computed using the spectral model employing the Lucey 1998 optical constants. The difference in trends is an important contributor to the error in prediction of modal mineralogy.
Figure A3. Black squares are the LSCC soils with a regression fit to the data. The diamonds are the locations of spectra computed using the spectral model employing the modified optical constants produced for this project. There is much better overlap between the predicted and measured spectra, and the trends produced by the two data sets.