

**AUTOMATIC ENDMEMBER SELECTION AND NONLINEAR SPECTRAL UNMIXING OF TERRESTRIAL MINERALS.** D. Rommel<sup>1</sup>, M. P. Felder<sup>1</sup>, A. Grumpe<sup>1</sup>, U. Mall<sup>2</sup> and C. Wöhler<sup>1</sup>, <sup>1</sup>Image Analysis Group, TU Dortmund University, D-44227 Dortmund, Germany; {daniela.rommel | marian.felder | arne.grumpe | christian.woehler}@tu-dortmund.de, <sup>2</sup>Max Planck Institute for Solar System Research, Max-Planck-Str. 2, 37199 Katlenburg-Lindau, Germany; mall@mps.mpg.de

**Introduction:** Recent development in hyper-spectral remote sensing has dealt with the advanced mineralogical analysis of the surface by spectral unmixing (e.g. [1]). Commonly, due to the lack of ground truth data, spectral unmixing is applied to a certain data set, and the results are discussed (e.g. [2]). The goal of this study is the generation of laboratory ground truth samples of known mineral composition in order to evaluate a nonlinear unmixing algorithm, in the context of unmixing analysis of lunar spectra based on terrestrial analog materials.

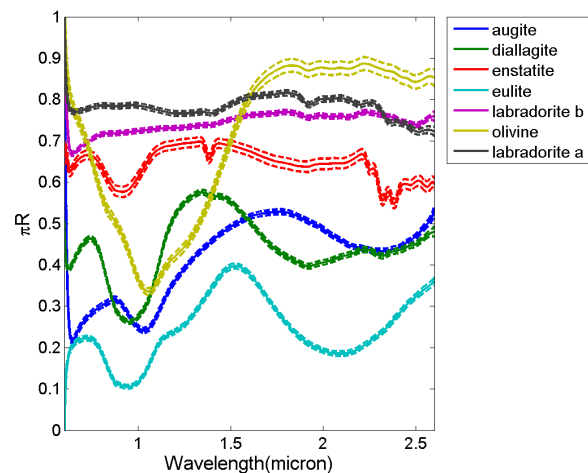
**Sample preparation:** For this study, we have used an endmember catalog of seven samples from different groups of minerals: augite, diallagite, enstatite, eulite, two labradorites and olivine.

**Powder generation:** All minerals were mechanically crushed and sieved to produce grains at various sizes, i.e. <32  $\mu\text{m}$ , 32-63  $\mu\text{m}$  and 63-125  $\mu\text{m}$ . Afterwards, impurities visible at microscopic inspection were removed by washing with solvents. Finally, the remaining impurities were removed manually.

**Mixture preparation:** In order to generate accurate mixtures, the corresponding powders were weighed using a high precision balance and mixed thoroughly by shaking the vessel containing all powders. Table 1 summarises the examined mixtures.

**Reflectance measurement:** The analysis within this work is restricted to a grain size of 32-63  $\mu\text{m}$ . All powders were filled into a circular sample container and flattened. The sample was illuminated by an HL-2000-FHSH halogene light source and the spectral radiance in the wavelength range 600-2600 nm was then obtained using an Arcoptix FTNIR-U-06-026 spectrometer. According to lunar remote sensing standard geometry [3], we apply a nadir view setup with an incidence angle of 30°. To derive the reflectance of the sample, the obtained radiance spectrum was divided by the radiance spectrum of a diffuse reflectance standard. The resulting reflectance spectrum is thus relative to that of an ideally white Lambertian surface. The normalised reflectance of the surface according to the Hapke model [4] is obtained by multiplication by the cosine of the incidence angle. For the pure minerals, six different sample containers were filled and each quadrant of the container was measured. The resulting 24 spectra are averaged to reduce the effects of different powder compressions and filling heights which may arise from different pressures during the manual flattening of the samples. Fig. 1 shows the averaged endmember spectra (solid lines) from our

catalog and the standard deviation over all 24 measurements (dashed lines). In case of the mixtures, two samples were measured at nine distinct spots.



**Figure 1:** Endmember catalogue. Solid lines: average endmember spectra. Dashed lines:  $\pm$  standard deviation

**Non-linear unmixing algorithm:** According to [5], nonlinear unmixing can be linearised based on the wavelength-dependent single-scattering albedo  $w$  of the Hapke model. We apply the full Hapke model including the anisotropic multiple scattering approximation [4, 6]. All parameters except the single-scattering albedo and the surface roughness parameter are adopted from [7]. The surface roughness is set to 0° due to the flattening during the sample preparation. The single-scattering albedo is then estimated by minimising the mean squared difference between the measured spectrum and the modelled reflectance for each spectral channel, respectively. The measured albedo spectrum is then linearly unmixed using albedo ( $w$ ) spectra of the catalog endmembers by minimising the mean squared differences between the measured and the mixed spectrum. Additionally, the sum of the endmember coefficients is constrained to a constant. The closed interval [0;1] is traversed in steps of 0.01, and the constant with the minimal error is chosen. This strategy accounts for model inaccuracies and measurement errors as well as agglutinate produced by spaceweathering [8] in the case of our planned examinations of lunar minerals.

**Endmember selection:** Due to the limited number of endmembers in the catalog, we apply an exhaustive search to select endmembers from the catalog. For each possible combination, a fitness function is evaluated, respectively. The fitness function is adopted from [9]. It sums the squared difference between the measured and the mixed albedo spectrum

and the squared difference of the corresponding continuum-removed reflectances. Additionally, spectral parameters, e.g. the position, depth and width of absorption troughs at  $\sim 1000$  nm,  $\sim 1300$  nm and  $\sim 2000$  nm, are computed and a normalised squared difference is added to the fitness function. Absorption features that are not present in the measured spectrum are penalised by adding a large constant.

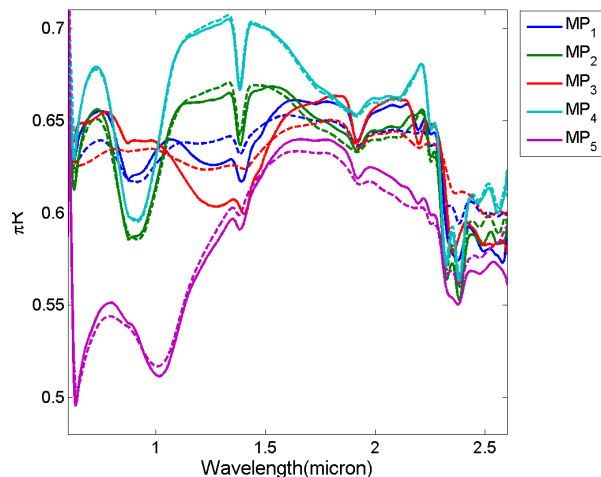
**Table 1:** Examined mixtures.

	mineral	wt%	mol%	estim. mol%
MP <sub>1</sub>	enstatite	30	30.6	25.6
	labradorite a	70	69.4	69.4
	olivine	0	0.0	0.5
MP <sub>2</sub>	enstatite	70	70.6	73.5
	labradorite a	30	29.4	24.2
	olivine	0	0.0	0.5
MP <sub>3</sub>	enstatite	10	10.2	0.0
	labradorite a	90	89.8	94.0
MP <sub>4</sub>	enstatite	90	90.2	88.5
	labradorite a	10	9.8	11.5
MP <sub>5</sub>	enstatite	30	30.0	26.5
	labradorite a	50	48.7	51.4
	augite	20	21.3	19.5

**Results:** The estimated mineral composition for each mixture, respectively, is given in Table 1. Notably, the estimated fractions do not sum to one. The remaining part may be interpreted as measurement uncertainty and absorbs possible modelling errors and/or different porosity caused by the manual flattening. The algorithm determines the correct endmembers. Only in case of MP<sub>1</sub> and MP<sub>2</sub> a negligible olivine fraction of 0.5 mol% is estimated.

The estimated fractions match the real fractions very well. The observed minor deviations may again be related to the reflectance modelling which influences the estimation of the endmember albedo spectra and the mixture albedo spectra. Thus, the results may be improved if multiple viewing and illumination geometries are considered.

Fig. 2 shows the reflectance spectra of the mixtures and the reconstructed reflectance spectra computed by the unmixing algorithm. The computed reflectance spectra of the estimated mixtures are in good agreement with the measured reflectance spectra. The mixture MP<sub>3</sub>, however, is not well represented by the pure labradorite spectrum. Furthermore, the prominent enstatite signature near 1000 nm is missing in the measured reflectance of the mixture. Hence, it appears to be difficult to determine the presence of enstatite if its fraction is only 10 wt%. At this point it is not clear whether the effect of the missing absorption is not modelled by the reflectance model or if it is just not present at the examined observation geometry.



**Figure 2:** Reflectance spectra of the mixtures (solid lines) and the reconstructed spectra of the unmixing result (dashed lines).

**Conclusion and Outlook:** We have shown that, in general, the Hapke model can be applied to transform the nonlinear unmixing problem into the problem of linear unmixing of the single-scattering albedo ( $w$ ) spectra. The obtained mineral fractions are in good agreement with the ground truth and show promising results. The endmembers were determined correctly from the available catalogue.

Further research will include the addition of further endmembers into the catalogue, e.g. ilmenite, which are known to have a strong influence on the reflectance of a mixture. Furthermore, the elemental composition of the catalogue minerals has been determined using electron microprobe analysis. Thus, the obtained mineralogical composition will allow for using to derive the elemental composition of the unmixed spectra.

The same experiments will be applied to measurements at different illumination and viewing directions to examine the influence of the illumination and derive an optimal set of incidence and emittance angles for the determination of the model parameters and the spectral unmixing result.

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**References:** [1] Keshava, N. and Mustard, J. F. *IEEE Signal Processing Magazine*, Jan. 2002, 44-57; [2] Heylen, R. and Gader, P. *IEEE Geoscience and Remote Sensing Letters*, in press; [3] Pieters (1999) *Workshop on New Views of the Moon II*, abstract #8025; [4] Hapke, B. (2002) *Icarus* 157(2), 523-534; [5] Mustard, J. F. and Pieters, C. M. (1989), *J. Geophys. Res.* 94, 13619-13634.; [6] Hapke, B. (1984) *Icarus* 59(1), 41-59; [7] Warell, J. (2004) *Icarus* 167, 271-286; [8] Mall, U. et al. (2012), *Geophysical Research Abstracts*, vol. 14, EGU2012-7852; [9] Felder, M. P. et al. (2013) EPSC Abstracts, vol. 8, EPSC2013-684.