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Supporting Information for

Spectroscopic characterization of impactites and a machine learning approach to determine the oxidation state of iron in glass-bearing materials

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Additional Supporting Information (Files uploaded separately)

Introduction

In the section **"Spectral parameters calculation"** we report the formulae for the calculation of band and spectral parameters discussed in the paper. We added more information about the building of the database in the section "**Additional notes on DB building**". For reader's convenience we report the plots for all the spectra acquired in this work. For two samples we report the variation of band center as a function of grainsize and the variation of the band center as a function of spectral slope (calculated between 400 and 2200 nm). For the smaller grainsizes in addition to the spectrum we also report

the continuum removed (cont_removed). All the spectra collected for this work are also reported in the attached spreadsheet "**ds01**". The database (DB) built from the data collected here and from literature work is made up of two spreadsheets: one spreadsheet (**"ds02"**) contains all ancillary information (chemical composition, grainsize, etc.) of the considered sample. For each sample we specified the reference from which we extracted the data so as additional steps (digitization and resampling where needed). This additional notes and references can be found in the second sheet named ("References_and_notes"). The spectra for all the considered samples are stored in a second spreadsheet ("**ds03**"). This spreadsheet is composed of several sheets, one for each paper from which we extracted the spectra. Each column header is the name of the sample and the corresponding ancillary information can be found on the first spreadsheet "info_DB" under the same sample's name.

Spectral parameters calculation.

After continuum removal we considered several spectral parameters to describe quantitatively our results. The spectral and band parameters considered here are band center (BC), band depth (BD), band area (BA), band centroid (BT) and spectral slope. The band center (BC) is the position of the band minimum in wavelength space while the band depth is the difference between the continuum reflectance and the band reflectance at the wavelength corresponding to BC

$$BA = \sum_{i=1}^{n} D_i \, \Delta x \qquad \textbf{(Eq.S 1)}$$

Where D_i is the amplitude (depth) of the band at the i-th wavelength (x) and $\Delta x = 1$ nm.

The band centroid was calculated according to (Eq.S *2*)

$$BT = \frac{\sum_{i=1}^{n} x_i D_i}{\sum_{i=1}^{n} D_i} \qquad \textbf{(Eq.S 2)}$$

Which corresponds to the weighted average of the band position (weight: amplitude). We also calculated the slopes of the spectra in several spectral ranges different from sample to sample. The spectral slopes are calculated with (Eq.S *3*)

$$SL = \frac{R_f - R_i}{WL_f - WL_i} \quad \textbf{(Eq.S 3)}$$

Where the R I s the reflectance and WL is the wavelength and the subscripts f and i (with $f > i$) to the wavelength at which the reflectance (R) is considered.

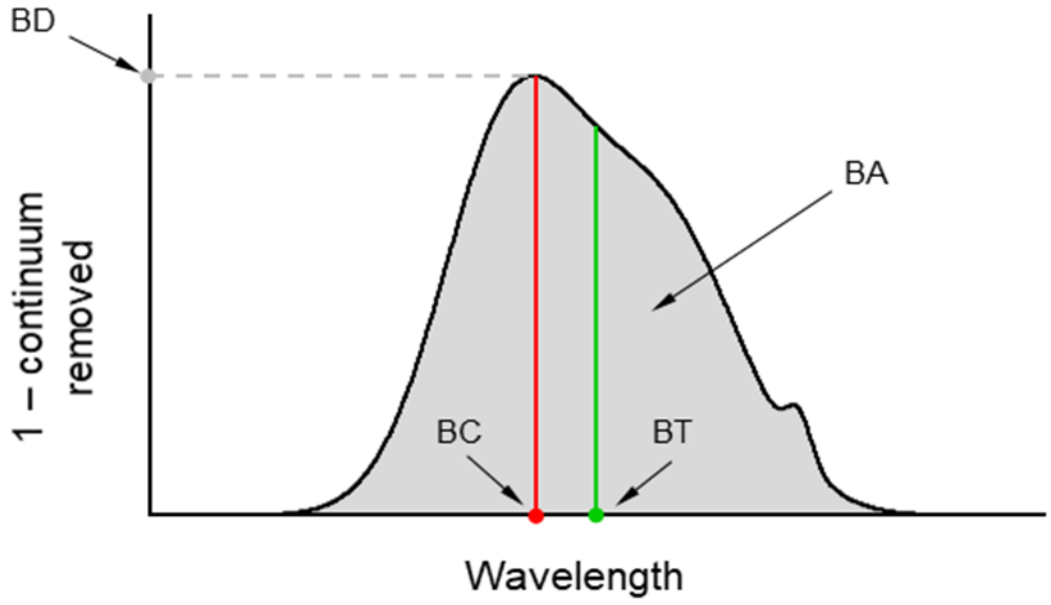

Figure S 1 Definition of the spectral band parameters used in this work

Additional notes on DB building.

To account for the spread in the grain sizes of the reported samples we calculated the standard deviation between the maximum and minimum size values of the grains in the powdered sample. We added the oxide composition of each sample in the database reporting, when possible, also the LOI values (loss on ignition, wt%). Several other parameters and spectral indices were calculated and added to the DB, namely: FeO+TiO_2, spectral slopes (between 400 and 2200 nm and between 500 and 1000 nm, average reflectance between 500 and 1000 nm (see Rader et al. 2022 for discussion about this parameter), ratio between the reflectance values at 415 and 750 nm, Fe^{3+}/Fe_{TOT}, temperature of closure (mainly for synthetic samples), constituent phases (glass, orthopyroxene, clinopyroxene, plagioclase, magnetite, groundmass) for each sample in volume % (if available). The chemical and physical information about each sample was stored in a

spreadsheet while in another spreadsheet we collected all the spectra for the samples present in the DB. Were the spectra were not available in electronic format they were digitized from the published plots. All the wavelengths are expressed in nm. Often it was necessary to interpolate the (literature) reflectance data and resample them to 1nm steps. The resulting body of information was then processed in Python 3 using a Jupiter Notebook running on a local machine. The two spreadsheets ("info_DB" and "spectra_DB") were imported into two different Pandas DataFrames . For the successive steps we only considered the data between 350 (wl_i) and 2400 (wl_f) nm. Finally, we merged the DataFrame containing the chemical and physical information with the DataFrame containing the binned spectra

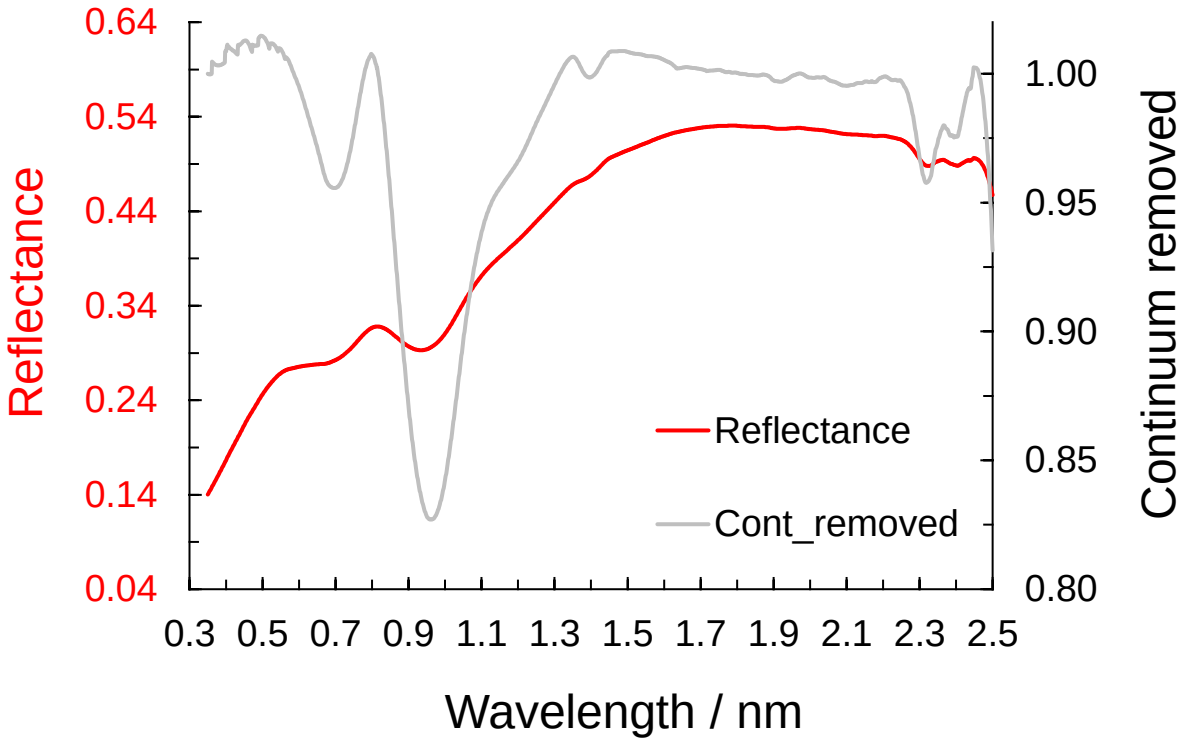

Figure S 2 Reflectance spectrum (0-25 µm size fraction) and relative continuum removed for the Dellen (D) sample. Note the wavelengths expressed as µm.

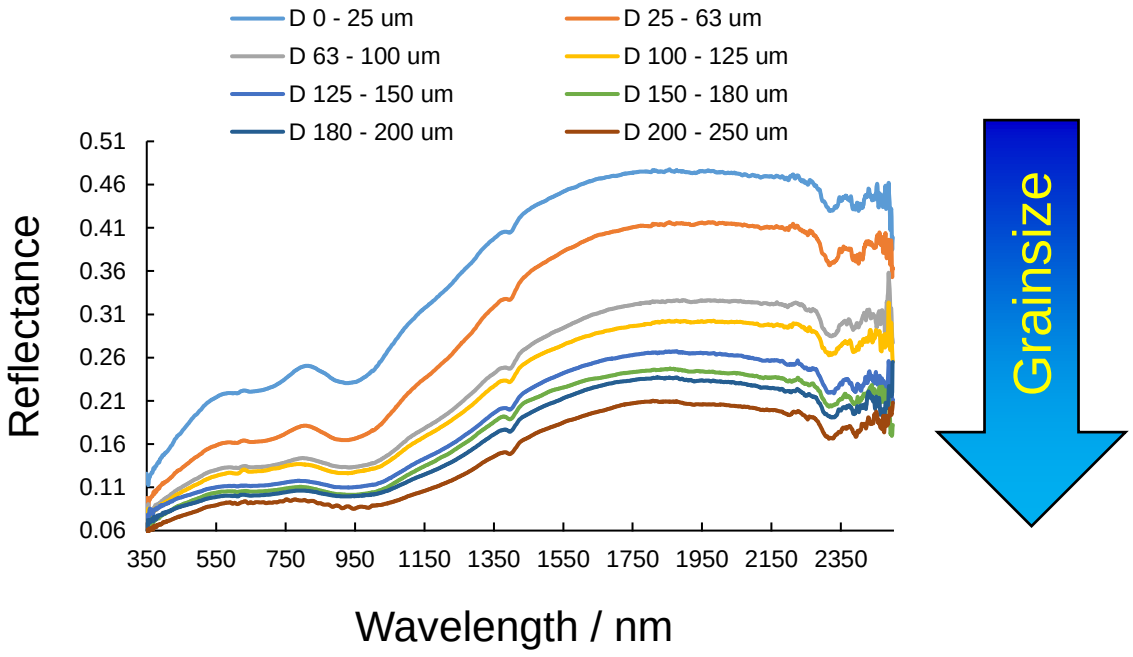

Figure S 3 Reflectance spectra for all the grainsizes classes of the D sample. The spectrum on top correspond to the 0-25 µm grain size while the one on the bottom is for the 225-250 µm. The spectra are not stacked. Wavelengths expressed an nm.

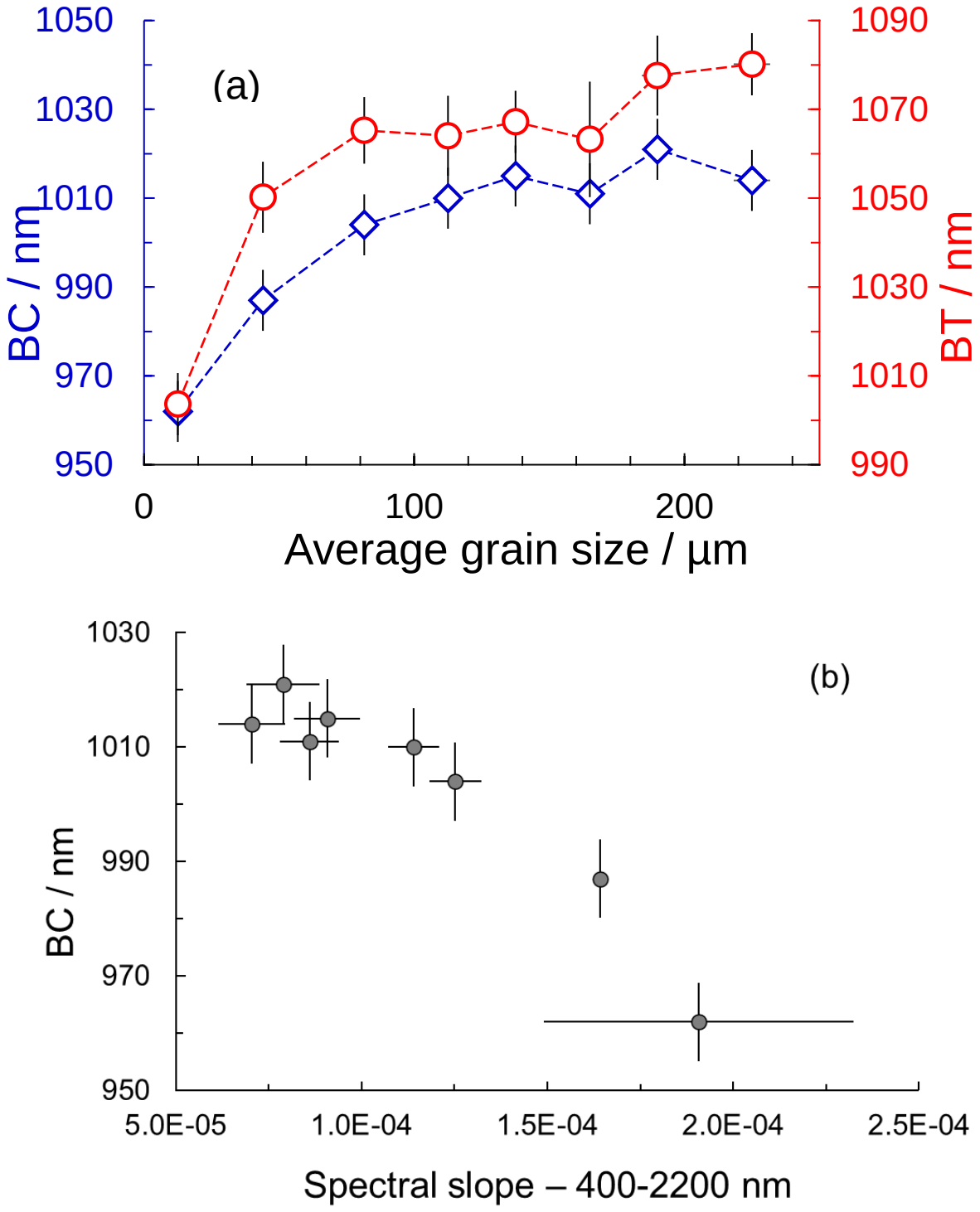

Figure S 4 a) Band center (BC – left y-axis) and band centroid (BT – right y-axis) as a function of mean grain size in Dellen (D) sample. b) BC as a function of spectral slope (calculated between 400 and 2200 nm) for the same sample

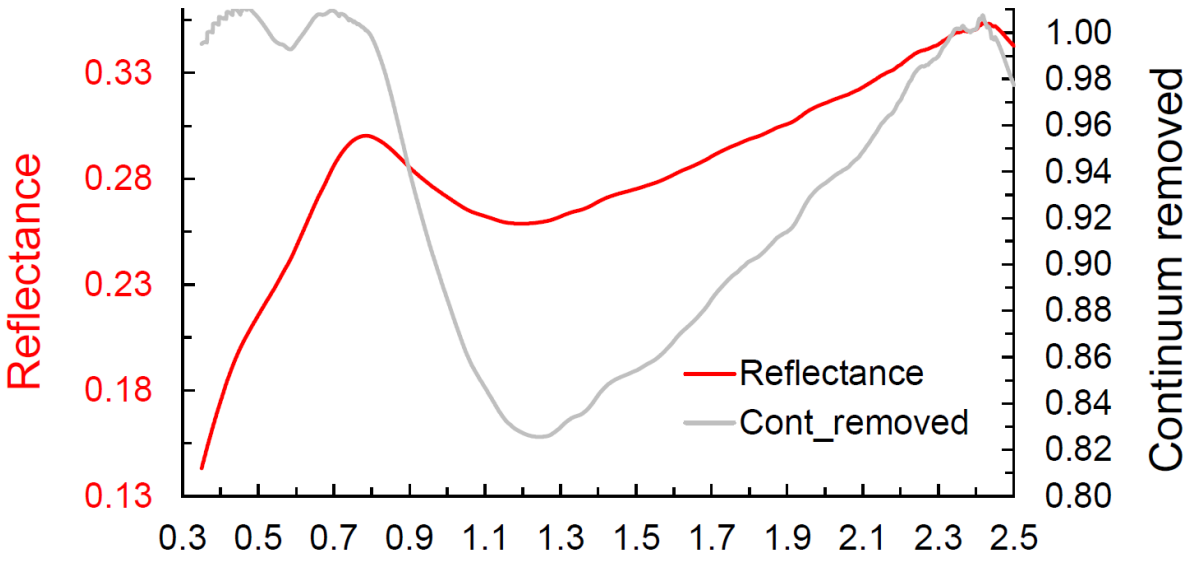

Figure S 5 Reflectance spectrum (0-25 µm size fraction) and relative continuum removed for the El'gygytgyn (E) sample. Note the wavelengths expressed as µm

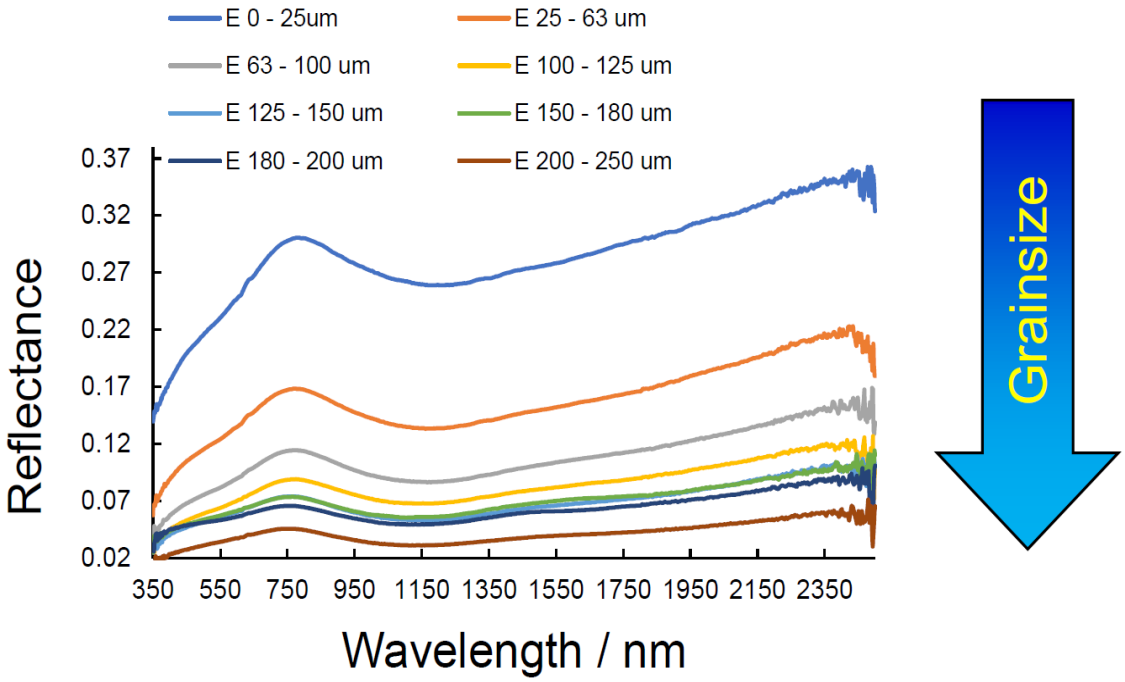

Figure S 6 Reflectance spectra for all the grainsizes classes of the E sample. The spectrum on top correspond to the 0-25 µm grain size while the one on the bottom is for the 225-250 µm. The spectra are not stacked. Wavelengths expressed an nm.

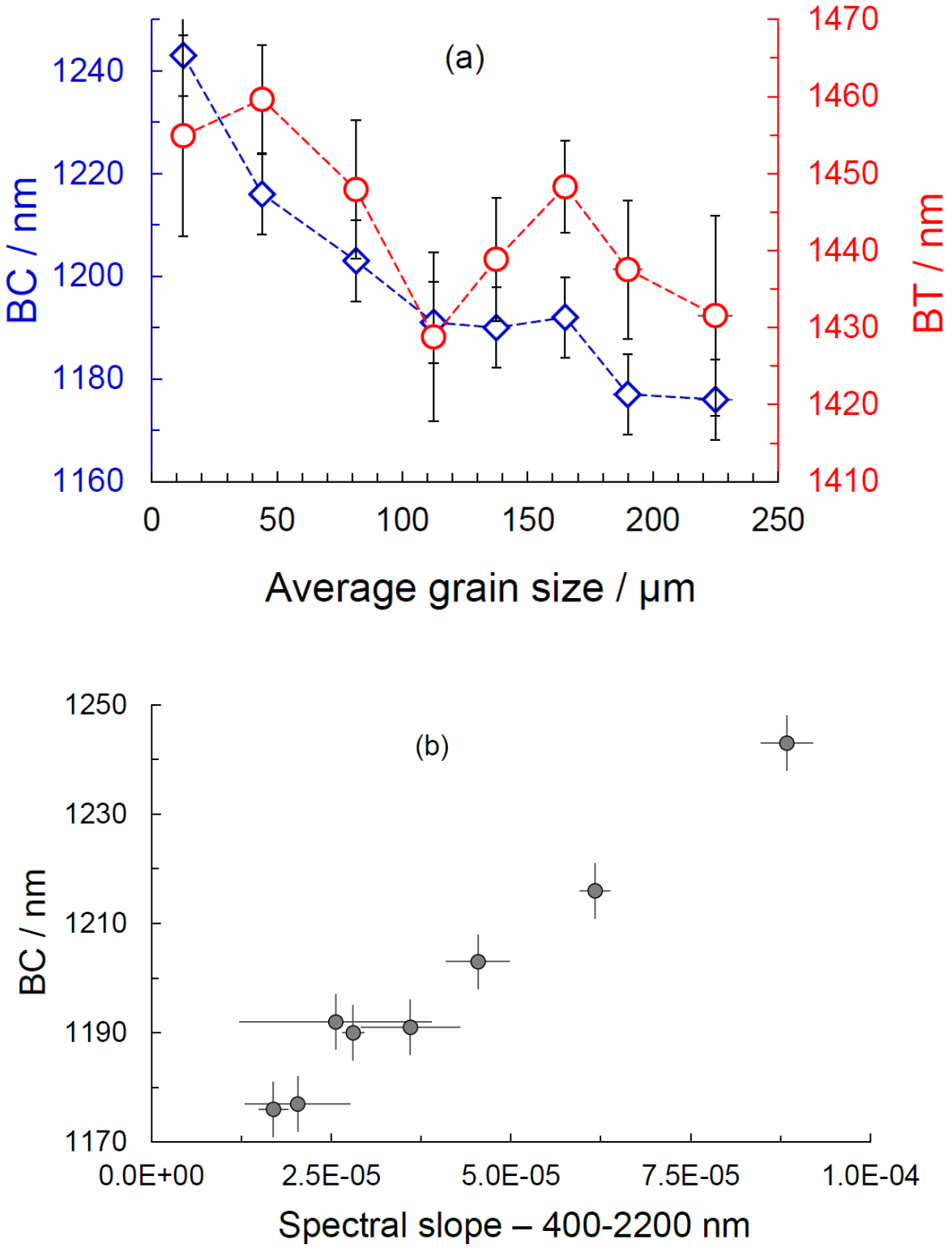

Figure S 7 (a) Band center (BC – left y-axis) and band centroid (BT – right y-axis) as a function of mean grain size in El'gygytgyn (E) sample. (b) BC as a function of spectral slope (calculated between 400 and 2200 nm)

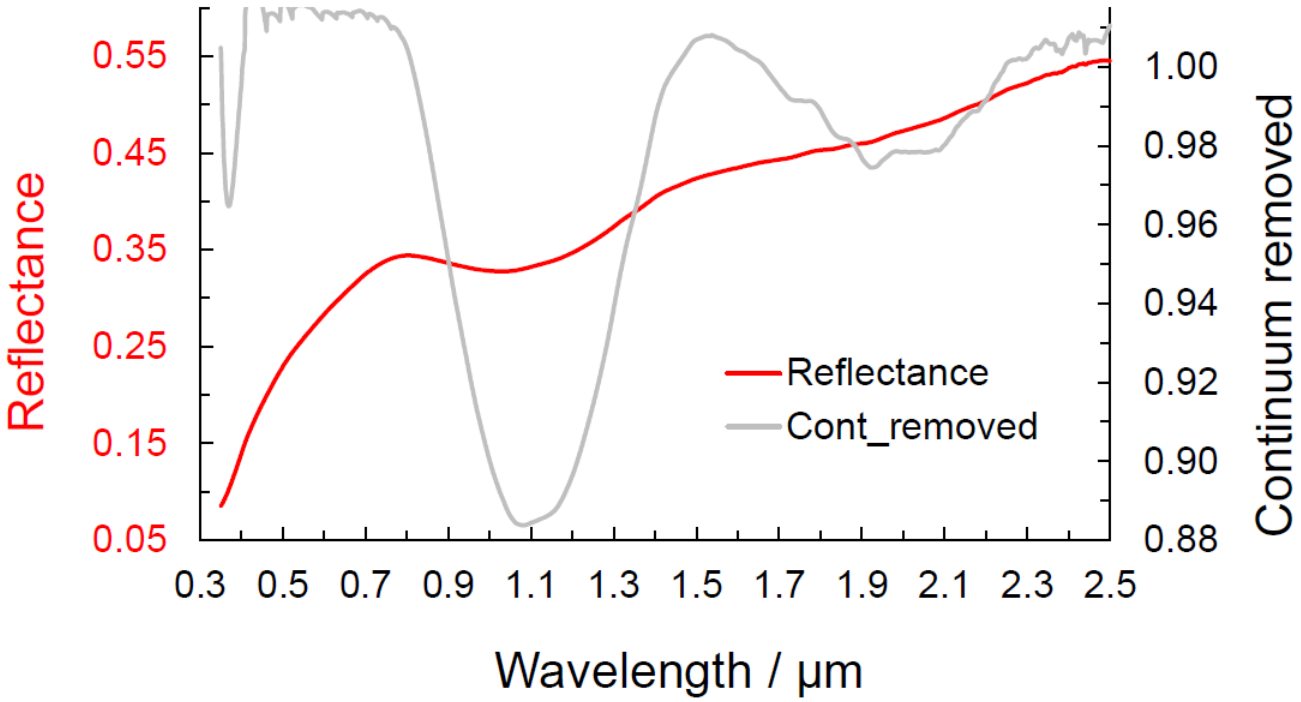

Figure S 8 Reflectance spectrum (0-25 µm size fraction) and relative continuum removed for the Irghizite (I) sample. Note the wavelengths expressed as µm.

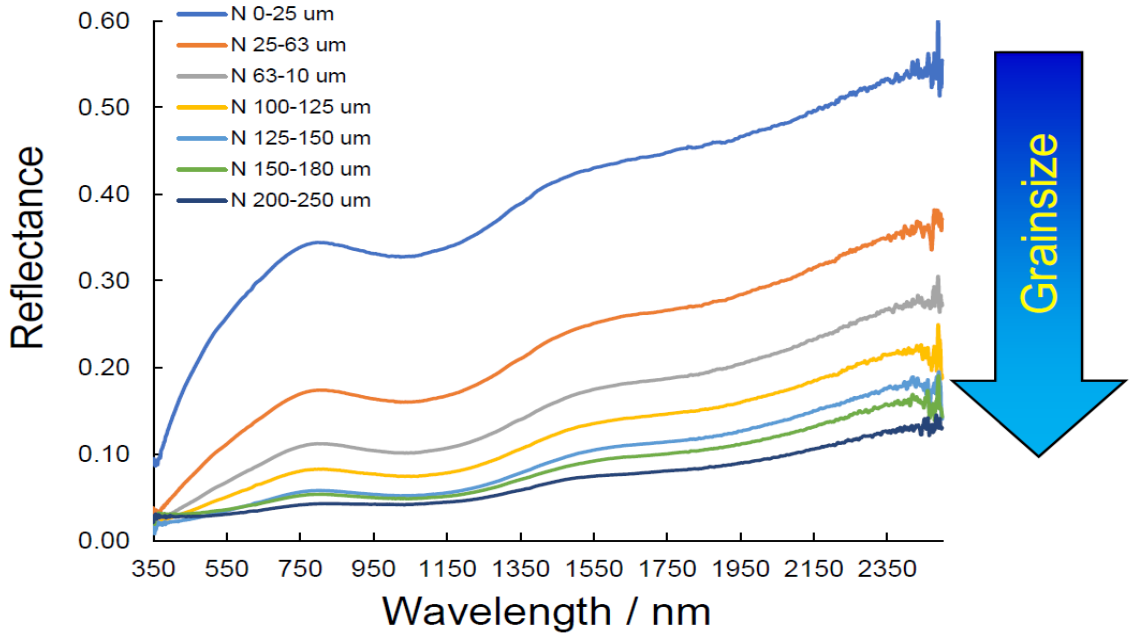

Figure S 9 Reflectance spectra for all the grainsizes classes of the I sample. The spectrum on top correspond to the 0-25 µm grain size while the one on the bottom is for the 225-250 µm. The spectra are not stacked. Wavelengths expressed an nm.

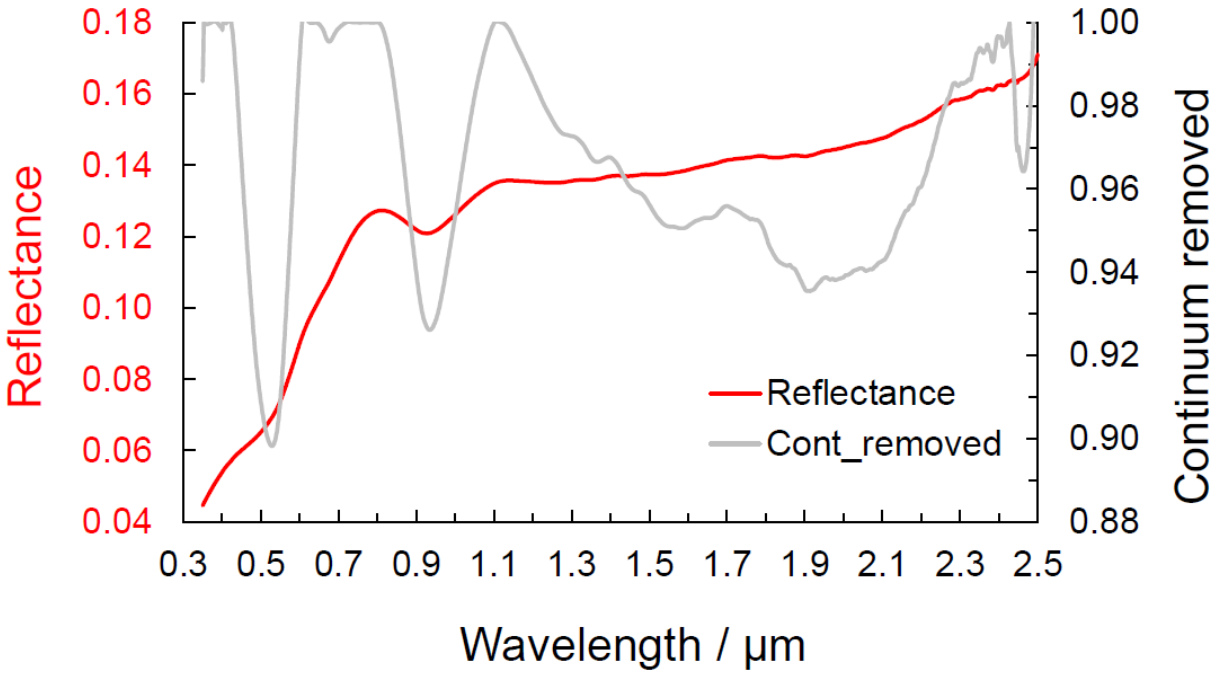

Figure S 10 Reflectance spectrum (0-25 µm size fraction; red left y-axis) and relative continuum removed (gray right y-axis) for the Lonar (L) sample. Note the wavelengths expressed as µm.

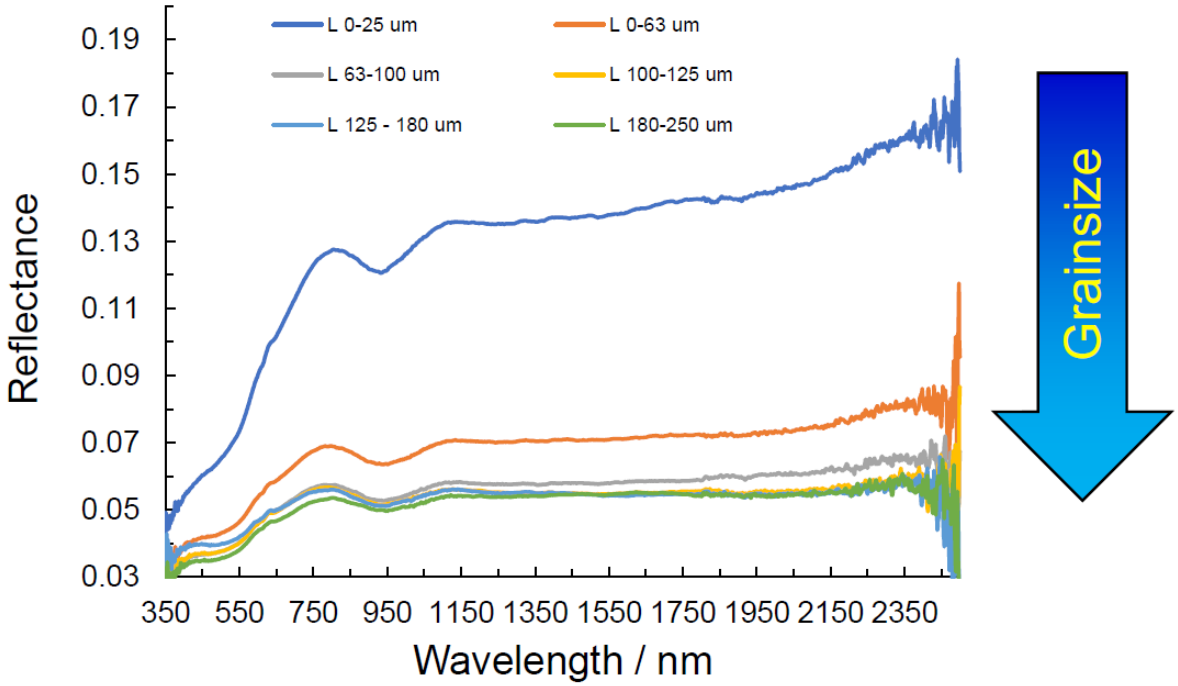

Figure S 11 Reflectance spectra for all the grainsizes classes of the L sample. The spectrum on top correspond to the 0-25 µm grain size while the one on the bottom is for the 180-250 µm. The spectra are not stacked. Wavelengths expressed an nm.

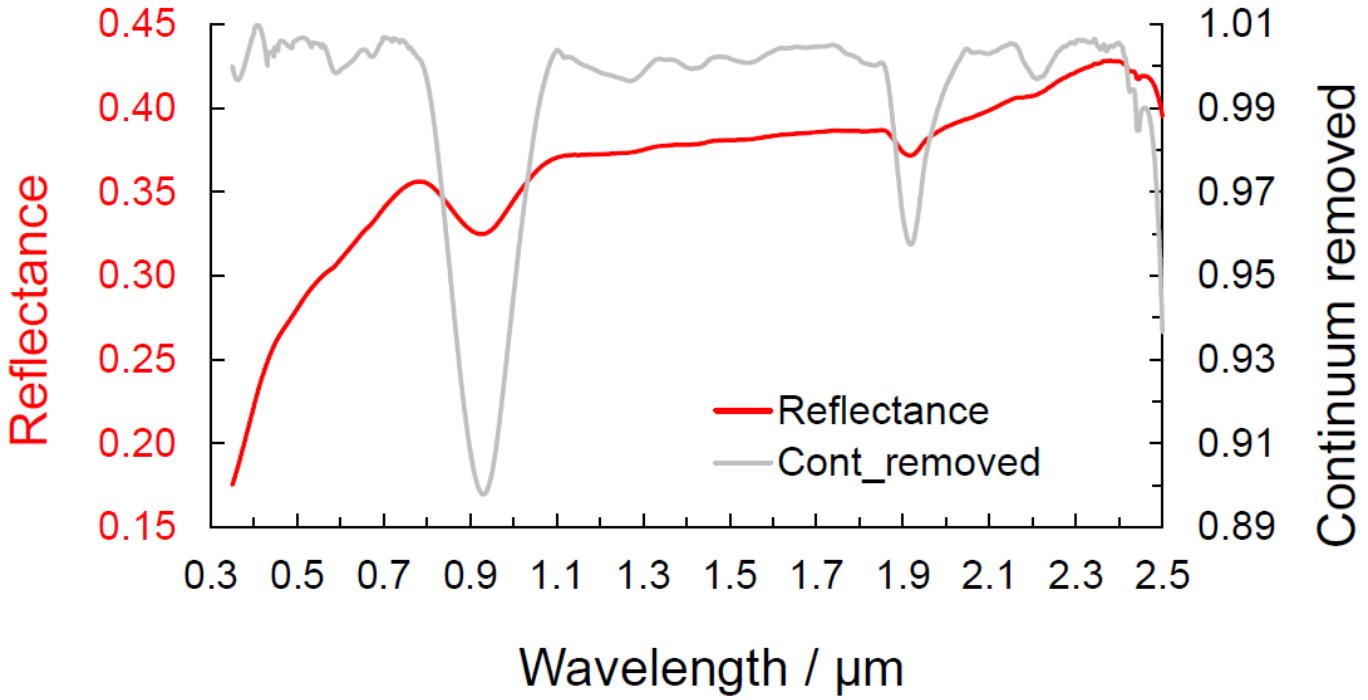

Figure S 12 Reflectance spectrum (0-25 µm size fraction; red left y-axis) and relative continuum removed (gray right y-axis) for the Mien (M) sample. Note the wavelengths expressed as µm.

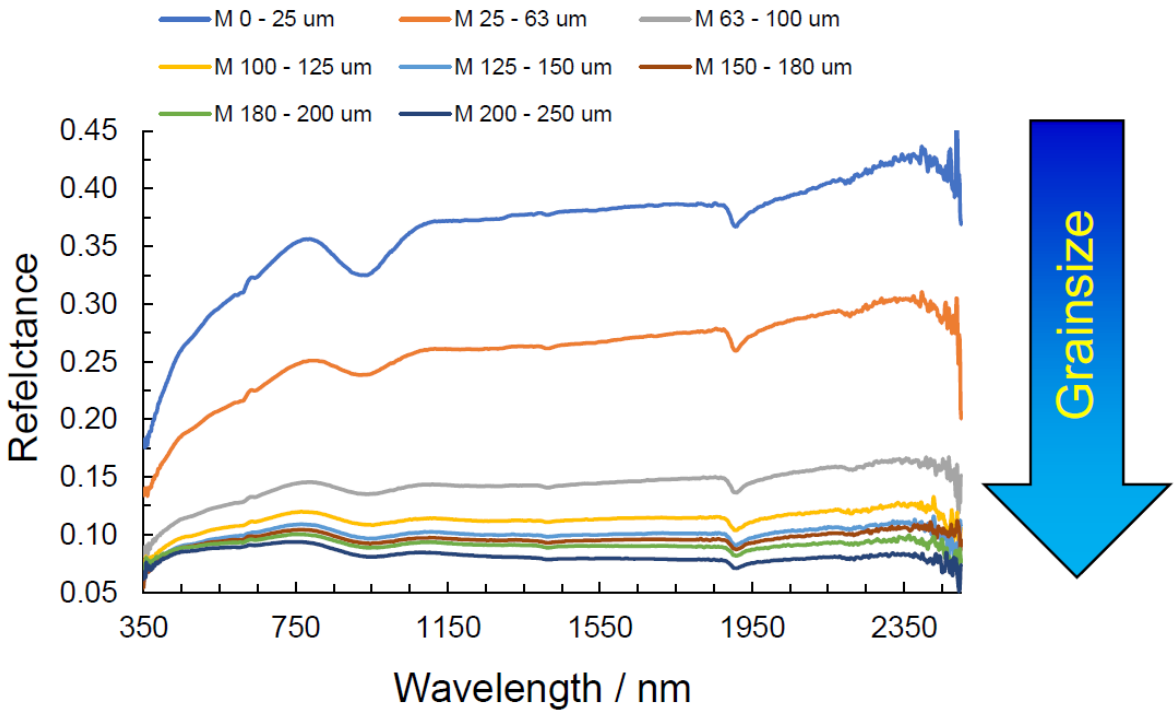

Figure S 13 Reflectance spectra for all the grainsizes classes of the L sample. The spectrum on top correspond to the 0-25 µm grain size while the one on the bottom is for the 180-250 µm. The spectra

are not stacked. Wavelengths expressed an nm. A small instrumental artifact is present between ~600 and 650 nm.

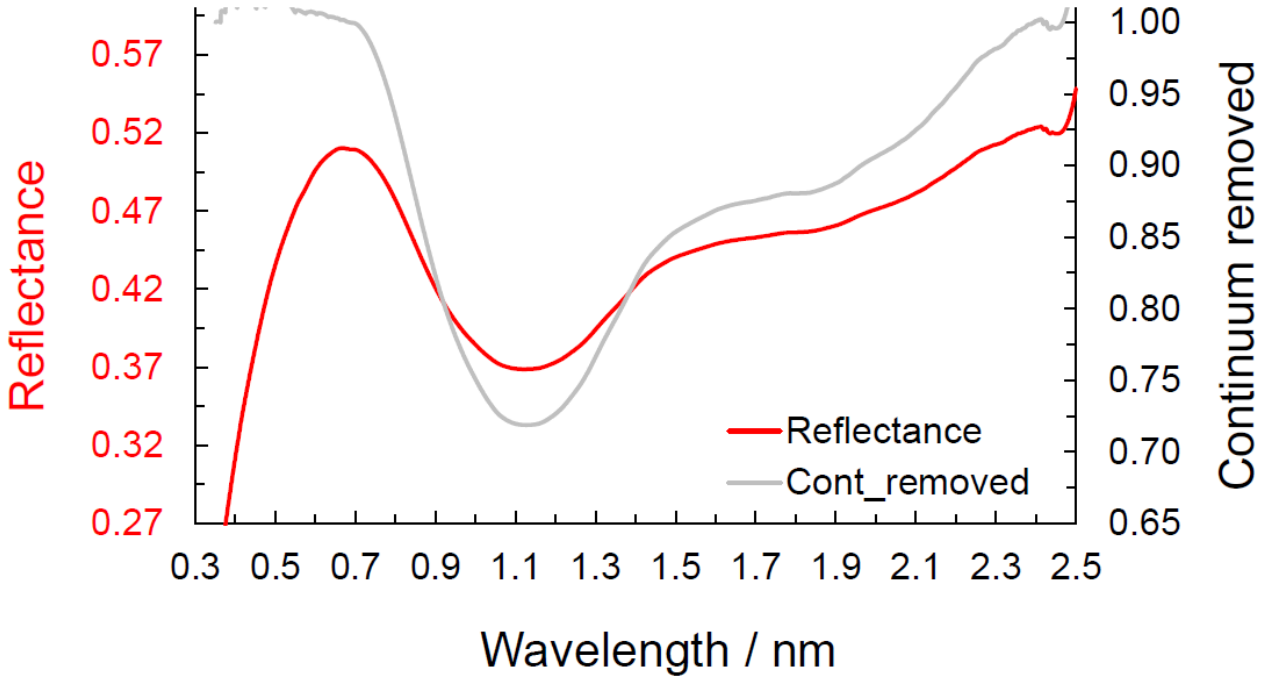

Figure S 14 Reflectance spectrum (0-25 µm size fraction; red left y-axis) and relative continuum removed (gray right y-axis) for the Muong-Nong (N) sample. Note the wavelengths expressed as µm.

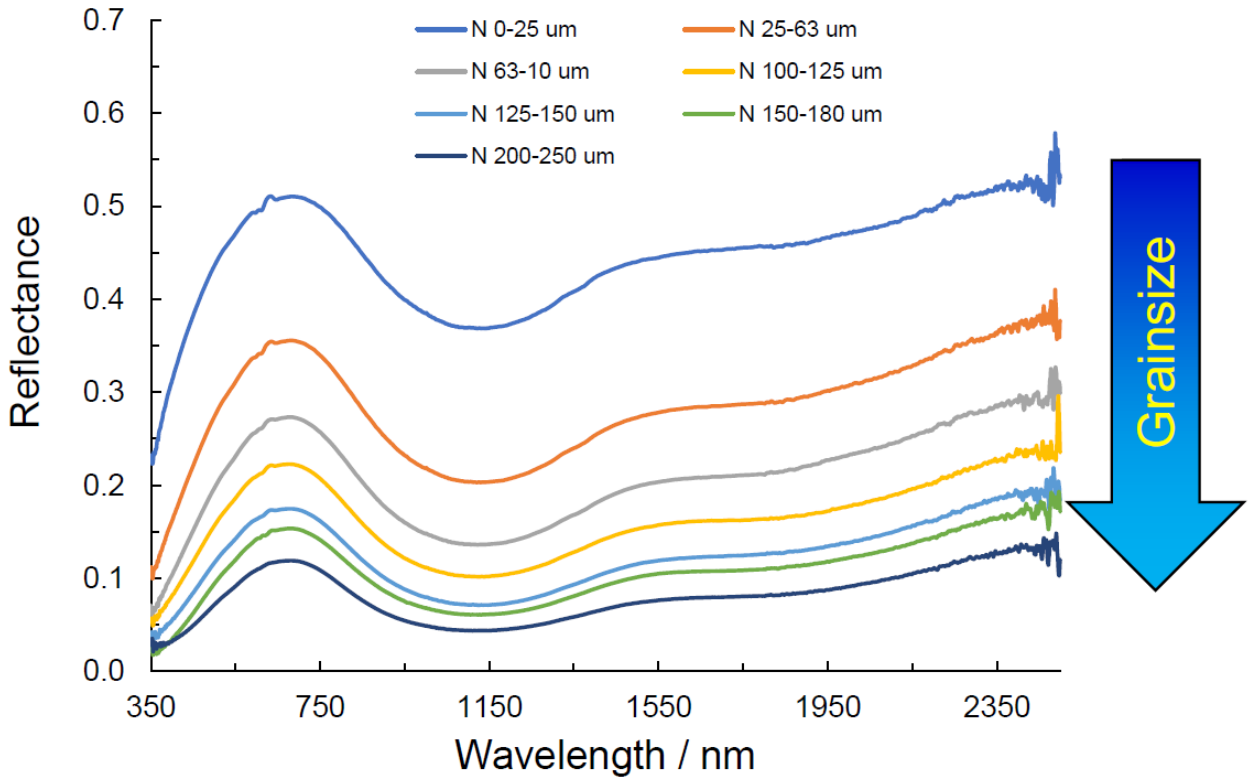

Figure S 15 Reflectance spectra for all the grainsizes classes of the N sample. The spectrum on top correspond to the 0-25 µm grain size while the one on the bottom is for the 200-250 µm. The spectra are not stacked. Wavelengths expressed an nm. A small instrumental artifact is present between ~600 and 650 nm.

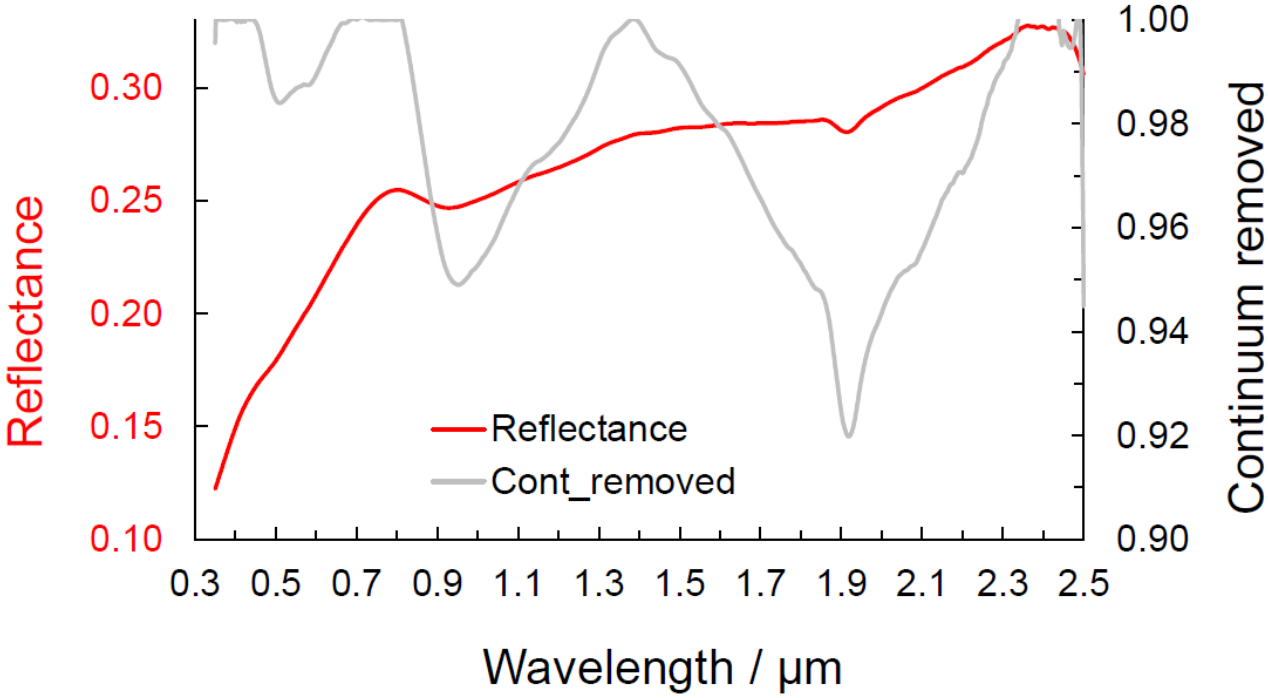

Figure S 16 Reflectance spectrum (0-25 µm size fraction; red left y-axis) and relative continuum removed (gray right y-axis) for the Popigai (P) sample. Note the wavelengths expressed as µm.

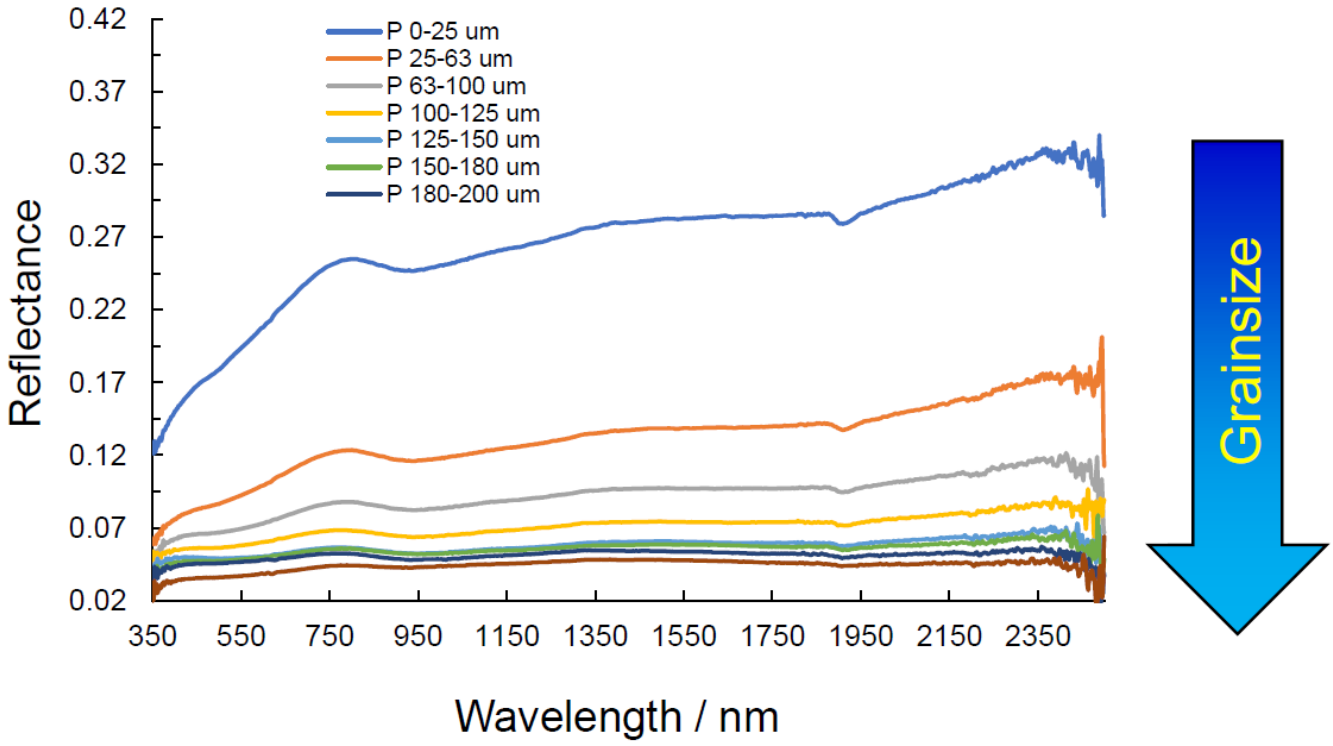

Figure S 17 Reflectance spectra for all the grainsizes classes of the P sample. The spectrum on top correspond to the 0-25 µm grain size while the one on the bottom is for the 200-250 µm. The spectra are not stacked. Wavelengths expressed an nm.

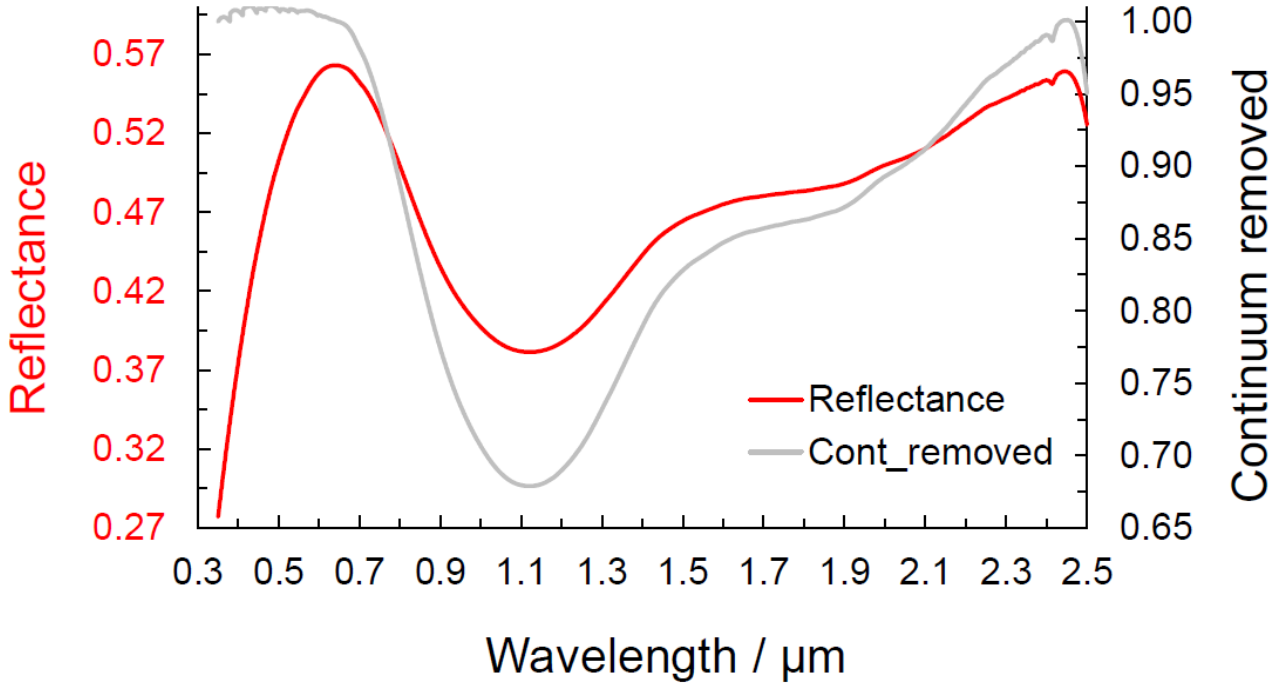

Figure S 18 Reflectance spectrum (0-25 µm size fraction; red left y-axis) and relative continuum removed (gray right y-axis) for the Thailandite (T) sample. Note the wavelengths expressed as µm.

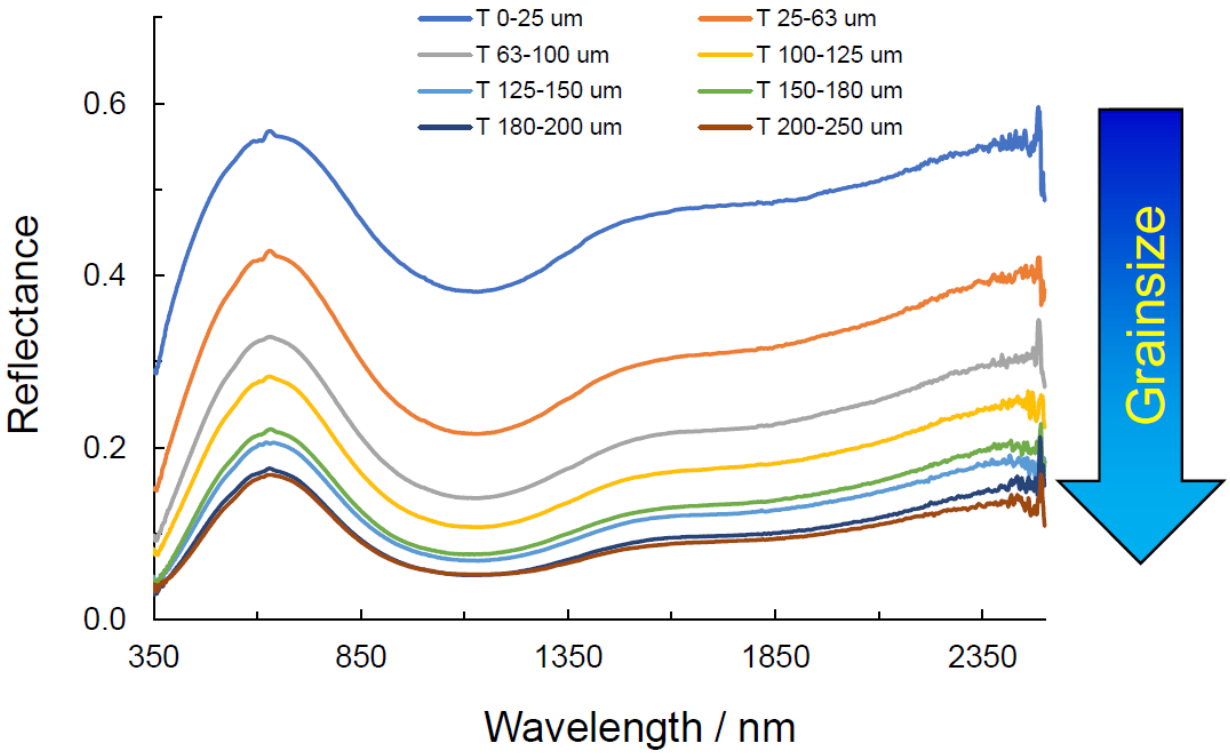

Figure S 19 Reflectance spectra for all the grainsizes classes of the T sample. The spectrum on top correspond to the 0-25 µm grain size while the one on the bottom is for the 200-250 µm. The spectra are not stacked. Wavelengths expressed an nm. A small instrumental is present between ~600 and 650 nm.

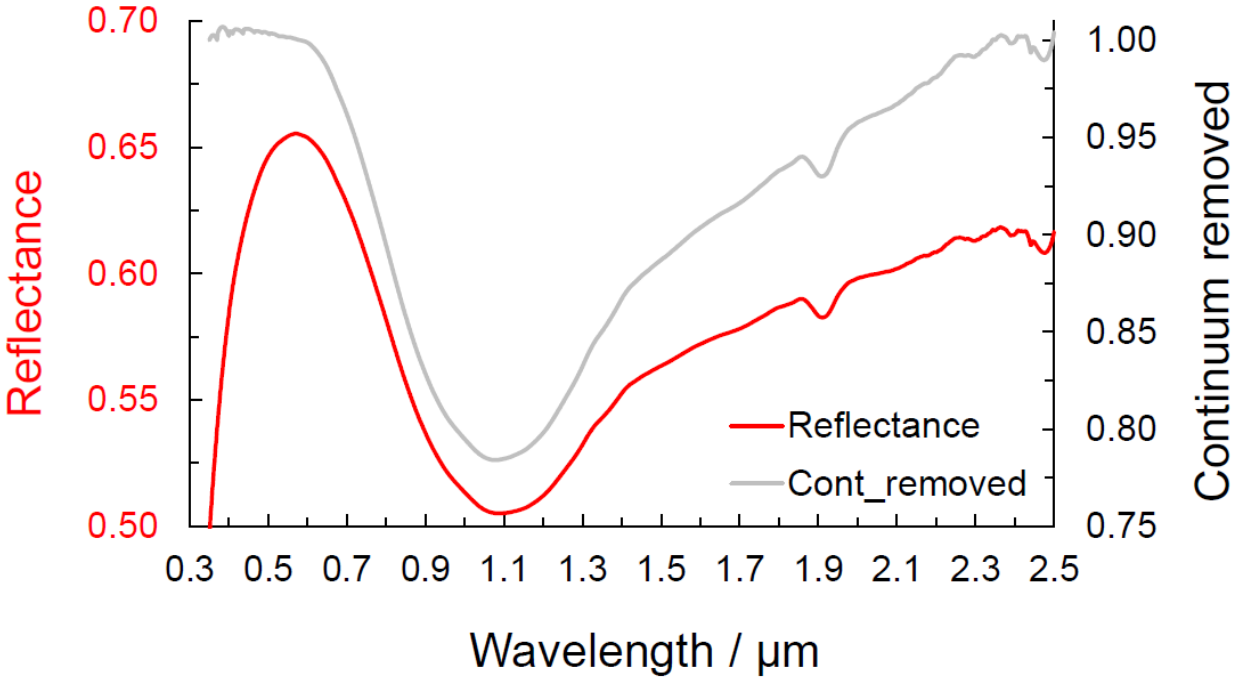

Figure S 20 Reflectance spectrum (0-25 µm size fraction; red left y-axis) and relative continuum removed (gray right y-axis) for the Moldavite (V) sample. Note the wavelengths expressed as µm.

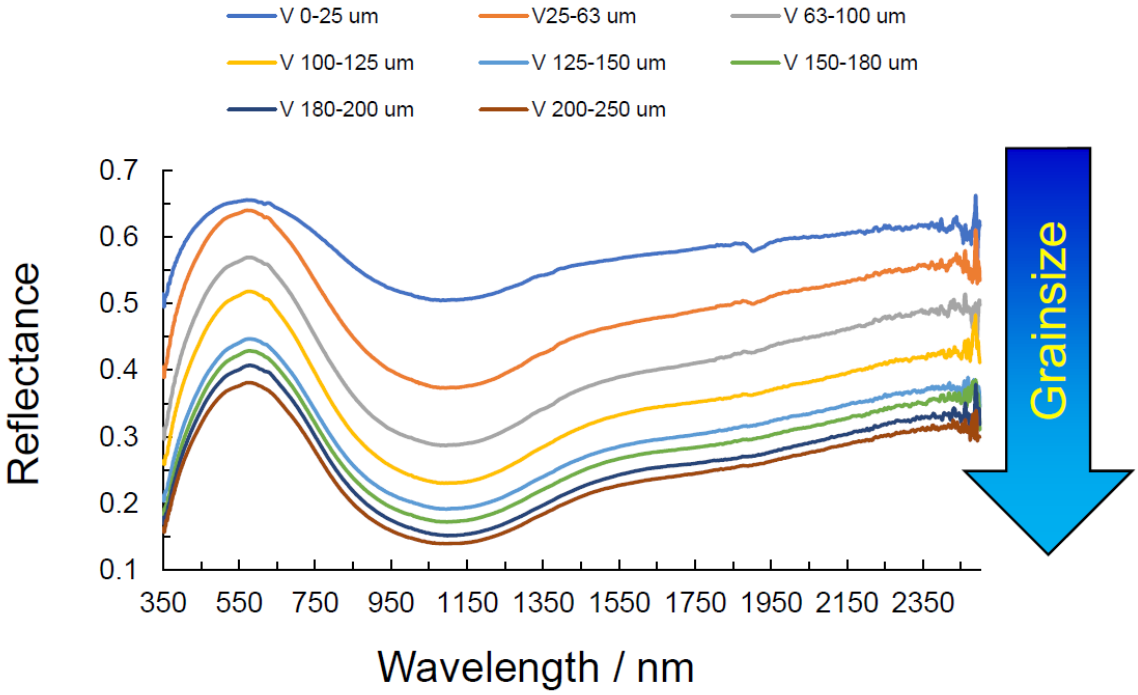

Figure S 21 Reflectance spectra for all the grainsizes classes of the V sample. The spectrum on top correspond to the 0-25 µm grain size while the one on the bottom is for the 200-250 µm. The spectra are not stacked. Wavelengths expressed an nm.

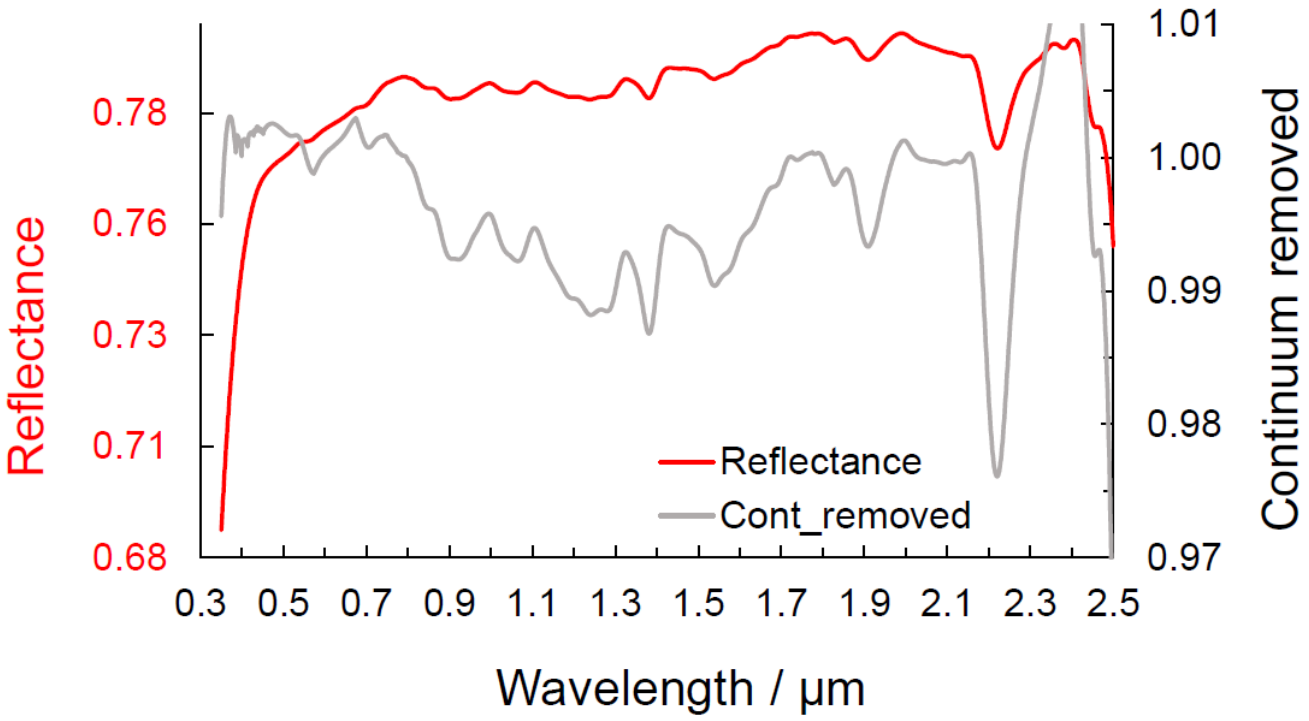

Figure S 22 Reflectance spectrum (0-25 µm size fraction; red left y-axis) and relative continuum removed (gray right y-axis) for the Libyan desert glass (W) sample. Note the wavelengths expressed as µm.

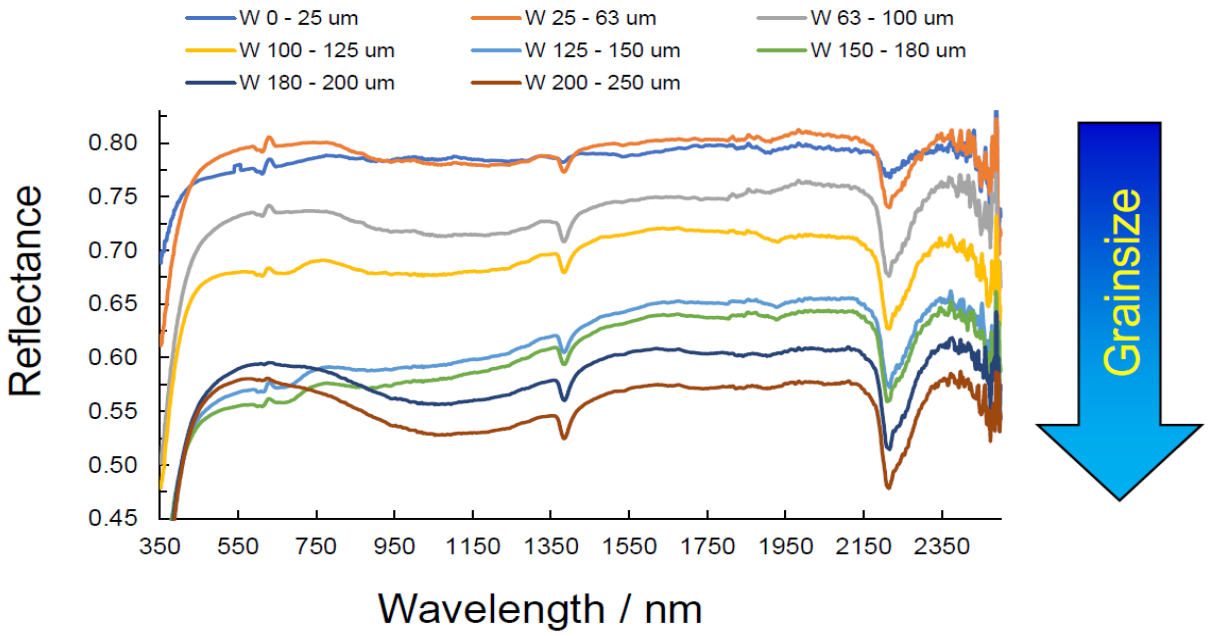

Figure S 23 Reflectance spectra for all the grainsizes classes of the V sample. The spectrum on top correspond to the 0-25 µm grain size while the one on the bottom is for the 200-250 µm. The spectra are not stacked. Wavelengths expressed an nm. A small instrumental artifact is present between ~600 and 650 nm

Data Set S1 (ds01). Reflectance spectra reported in this work. For each sample all the grainsizes are reported. The spreadsheet contains standard deviation for each channel (wavelength), smoothed spectra, continuum and continuum removed spectra.

Data Set S2. (ds02) There are two spreadsheets: "info_glasses" with all the ancillary information about the samples used in the database and "References_and_notes" with the complete literature references and the information about data processing (if any)

Data Set S3. (ds03) The file is made up of 8 sheets each of which contains all the spectra relative to a given literature work identified by the first name's author and publication year (references can be found on the main article). All the spectra are reported in wavelength (nm)

Data Set S4. (ds04) The file is the Jupiter Notebook containing the machine learning code discussed in the paper

Data Set S5. (ds05) Same as "ds04" but with the usual Python extension .py

Table S1. Band parameters for the investigated samples. Sample's names are as follow: J_ll_hl where J is the sample acronym, ll: lower limit (μm) for the granulometric class and hl is the higher limit (μm) of the granulometric class. BC is the band center (position in wavelength space of the deepest point of the band after continuum removal; see supplementary materials); BD is the band depth; BA is the band area and BT is the band centroid. Bands are numbered in increasing order (the band whose center is at lowest wavelength is band nr. 1)

Table S2. Powder X-ray diffraction results of the studied samples