

Advanced mgm deconvolution on powder versus slab of olivine natural samples: a test with nwa 5400

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Introduction: As shown in [1], the use of MGM modeling, with the handling of the overall continuum by a second-order polynomial initially adjusted on the main maxima along the reflectance spectrum, is a clear progress. This approach is close to the convex hull one, but is more flexible in the sense that it does not constrain the continuum to be tangential to the spectrum though it does not preclude it. Continuum slopes are well known to be highly variable, being affected by a number of parameters, which include surface texture, grain size, viewing geometry, and alteration due to space weathering. The results which are produced, all particularly with natural samples, suggest that the continuum physical understanding hides additional complexity yet to be explored. The robustness of the proposed solution is also significantly increased by the use of a fixed set of starting conditions able to address situations ranging from laboratory to orbital data.

The band center positions of the three primary olivine absorptions (M1-1, M2, M1-2) are used simultaneously to produce a constrained prediction across an extended forsterite range Fo#[0-90] of olivine solid solution composition. The established trend lines based on synthetic samples with composition ranging from Fo#0 to #90 appear robust when implemented on controlled natural samples, and represent an improvement over previous solutions.

However, the validation has been mainly made so far on controlled powder samples with typical grain size less than 60 micron, and it remains to explore how this modeling behaves when implemented on rough-powdered and slab olivine-rich samples, in the context of natural cases involving multiple mineral phases. Natural samples can indeed be found with variable grain sizes or as rock slabs/chips and are likely not devoid of minor amount of cations such as Fe3+, Cr2+, Mn2+, Ca2+,... which may disturb the optical properties across the olivine composition range.

Case of a powder versus slab natural sample: To take a first step in this direction, an assessment is performed here on a well–characterized sample of NWA 5400 meteorite (a dense, dark brown, rounded stone (4818 g) partially covered with a weathered fusion crust), found in Algeria in 2008 [2]. Its petrographic description indicates a coarse-grained rock (grains mostly in the range 0.2–0.8 mm) with protogranular texture, composed predominantly of olivine (79vol%, Fo#~70) with subordinate orthopyroxene (10.5 vol%, Fs24.4Wo2.1), clinopyroxene (8.9 vol%, Fs9.4Wo45.1), chromite (1.4 vol%), Clrich apatite, troilite, kamacite (altered to iron hydroxides) and minor taenite. No plagioclase was observed despite a careful search. (see description of Northwest Africa 5400 in Meteoritical Bulletin) [3].

Powdered and slab samples have been prepared; the powders discussed hereafter have a grain size ranging between 0 and 100 μ m, with very few grains (less than 5 % in volume) with dimension larger than 100 μ m. Their reflectance spectra have been acquired in the 0.35-2.5 μ m domain on a spot size with a diameter of the order of 5-6mm by means of an ASD field spectrometer.Two spectra (powder and slab cases) are shown below.

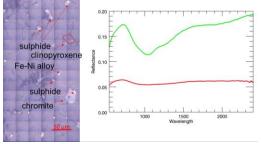


Figure 1. (*Left*) FTIR picture at microscopic scale in reflected light of a portion of the slab sample (minerals identified from SEM); (*Right*) NWA 5400 reflectance spectra on a powder sample shown in green and on a slab in red.

Olivine Spectra Deconvolution and results: An advanced MGM deconvolution process is then applied to these spectra. Among a number of tests, two results are shown and discussed below.

The deconvolution of the powder spectrum is first addressed. A set of 5 dedicated Gaussians (band center, band width, intensity and associated uncertainties) is used and referred to in the following as L5 reference configuration. The first Gaussian, centered around 450 nm, is used to model the strong large absorption at shorter wavelength (i.e. charge transfer towards the ultraviolet). The '650nm' Gaussian, though generally quite shallow, appears to handle absorptions possibly caused by transitions of minor elements such as Cr, Ni or by charge transfers of other elements. Both Gaussians also contribute stabilizing the overall shape of the continuum in the visible domain. The next Gaussians respectively centered at 850, 1050, 1250 nm and referred to as M1-1, M2, M1-2 address Fe²⁺ charge transfers absorptions.

As shown on figure 2, the modeling appears wellbehaved with a flat line residuals all along the spectral domain (rms: 0.0043). The '650nm' Gaussian has a rather pronounced band depth consistent with the Cr presence in the sample.

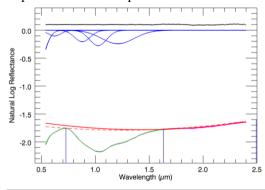


Figure 2. NWA 5400 powder spectrum MGM deconvolution. Measured spectrum (pink line) and MGM modeled one (green solid line) with the Gaussians (solid blue lines) and polynomial (dashed -starting continuum- and solid -final continuum after running MGM- red lines) and the residuals line in black along the spectral domain. For clarity, the residuals (observed - modeled quantity) are shifted by +0.1 which means that a perfect fit is displayed with a 0.1 flat line. Position of the local maxima (anchor points) along the spectrum used for the process of initialization shown by thin vertical blue lines (3rd anchor point not displayed if beyond 2.5 micron).

While the deconvolution of the powder spectrum gives classical enough outputs (see [1]), the spectrum of the slab sample (figure 3) has to be handled with a slightly different MGM configuration requiring two Gaussians in the SWIR and no '650nm' Gaussian. The spectral residuals are still low (rms:0.0048) though a bit more shaky. One notes that the M2 intensity is less than M1-1 which is not expected when modeling a pure olivine phase and calls for the contribution of other phases or the presence of minor amounts of various cations (Ca²⁺, Mn²⁺, Cr²⁺, Fe³⁺,...) disturbing the olivine characteristic absorption features.

However, despite these complexities, the prediction of the olivine composition based on the minimum deviation from the three trend lines established in [1] gives the following Fo# estimates : 75 for the powder case; 67 for the slab case (see figs. 4 and 5).

Conclusions: Despite the heterogeneity of the sample in this natural context, the olivine composition prediction, though affected by the presence of additional phases, is for both powder and slab cases, close to the actual Fo#~70.

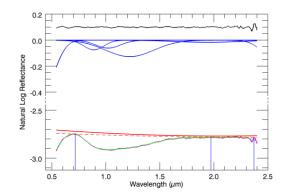


Figure 3. NWA 5400 slab spectrum MGM deconvolution (see Fig.2 for figure caption).

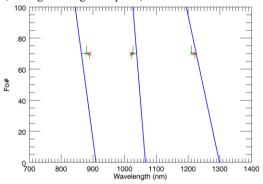


Figure 4. Compositional trend lines from [1] in blue in molar Fo# versus band center (nm). Crosses (x) plot for both (powder x and slab x) samples the actual Fo# associated with M1-1, M2, M1-2 band centers determined by MGM deconvolution (see figs. 2 and 3). The horizontal thin bars display the real distances to trend lines while the vertical thin bars show predicted-actual Fo# quantities.

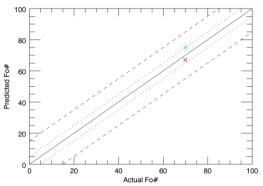


Figure 5. Predicted versus actual molar Fo# estimates. x cross for powder, x cross for slab case.

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