

REASSESSING THE RELATIONSHIP BETWEEN OLIVINE COMPOSITION AND REFLECTANCE SPECTROSCOPY FROM ADVANCED MGM DECONVOLUTION. P.C. Pinet^{1,2}, S.C. Chevrel^{1,2} and Y.H. Daydou^{1,2}. ¹Université de Toulouse; UPS-OMP; IRAP; Toulouse, France, ²CNRS/CNES; IRAP; 14, avenue Edouard Belin, F-31400 Toulouse, France (patrick.pinet@irap.omp.eu).

Introduction: We revisit the behavior of the three primary olivine absorptions near 1 μm (referred to as M1-1, M2, M1-2) and their interrelationships by means of an advanced version of MGM analysis. We build on the previous works carried out [e.g., 1,2] to document at best the compositional variation of olivine from diagnostic absorption features across the visible and near-infrared wavelengths due to electronic transitions of Fe²⁺ in the crystal structure.

MGM implementation: The principle of the Modified Gaussian Model is to deconvolve overlapping absorptions of mafic mineral spectra into their fundamental absorption components. Its specific interest is to directly account for electronic transition processes[e.g., 3]. The MGM approach is in essence able to achieve a direct detection and quantification of minerals. It is achieved by considering a sum of modified Gaussian functions characterized by their band centers, widths, and intensities. Spectra are modeled in the logarithm of reflectance space as a sum of modified Gaussian distributions superimposed on a baseline continuum. The resulting combinations of Gaussians can then be interpreted in terms of mineralogy. However, as demonstrated by [4, 5], MGM results are sensitive to the initial parameters (i.e., centers, widths, and intensities) and a key issue is to properly initialize the MGM parameters [5]. Consequently, an automatic analysis of the shape of the spectrum is first performed (spectrum maxima and minima are used to estimate at first order absorption strengths and widths). In the following, at the difference of a number of previous studies, the continuum is handled with a second-order polynomial initially adjusted on the local maxima along the reflectance spectrum (curvature, slope, and shift are free to move during the modeling). This is achieved by means of three anchor points searched within three spectral windows respectively spanning the intervals: 450-850, 1300-2000, 2300-2600nm. The robustness of modeling is also significantly increased with a set of starting conditions able to address situations ranging from laboratory to orbital data [5, 6, 7]. For the olivine MGM modeling, a set of 4 dedicated Gaussians (bandcenter, bandwidth, intensity and associated uncertainties) is used. The '650nm' Gaussian, though generally quite shallow, appears to handle

absorptions possibly caused by transitions of minor elements such as Cr, Ni or other charge transfers.

Gaussian	Center (nm)	Width (nm)	intensity
'650'	650+/-150	150+/-300	-0.25+/0.5
M1-1	850+/-200	250+/-500	-0.25+/0.5
M2	1050+/-200	200+/-500	-0.25+/0.5
M1-2	1250+/-200	450+/-500	-0.25+/0.5

Olivine Spectra Deconvolution / Methodology:

MGM inverse modeling provides with band center, band width and band depth estimates. Band centers are used to determine trend line equations for each individual absorption band, with an assessment on the regression performance (rms spectral distance between bandcenter estimate from MGM and the one from the trend line). The olivine composition (Molar Forsterite Fo#) is then predicted based on minimizing the deviations in band centers from the established trends for the three absorptions simultaneously, using the integrated rms spectral distance to trend quantity (**sdt**).

Synthetic olivine samples. A careful selection from [3] leads to a suite of 6 controlled and well-characterized synthetic olivine samples [2, 8] that can be considered to be the best examples of pure olivine for which the spectral optical properties are unaffected by the inclusion of minor cations. These samples, referred to as suite 1, span the range of Fo#0 to 70. Our MGM approach is thus first implemented on this suite of spectra, referenced as table 6 in [2], and then extended (suite 2) to the range of Fo#0 to 90, using 10 synthetic samples. Fo#20 case is shown below (Fig. 1).

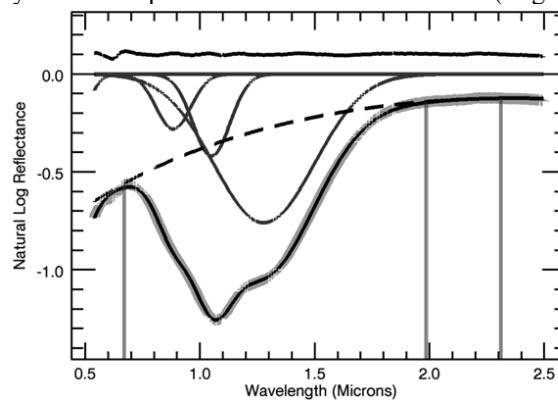


Figure 1. Case of C1DD96 (Fo#20). Measured spectrum (light grey crossed line) and MGM modeled one (thick black solid line) with the Gaussians (solid black lines) and polynomial (hatched line) and the residuals line along the spectral domain. Position of the local maxima along the spectrum

used for the process of initialization (anchor points found at 670, 1985, 2310nm). 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 (rms : 0.005).

A systematic testing of the coherency is performed to assess the performance of each regression. For suite 1, the integrated Fo# rms deviation is 4.5, with a 6 nm rms sdt. For suite 2, the integrated Fo# rms deviation is 4.8, with a 6.5 nm sdt (see Fig. 2).

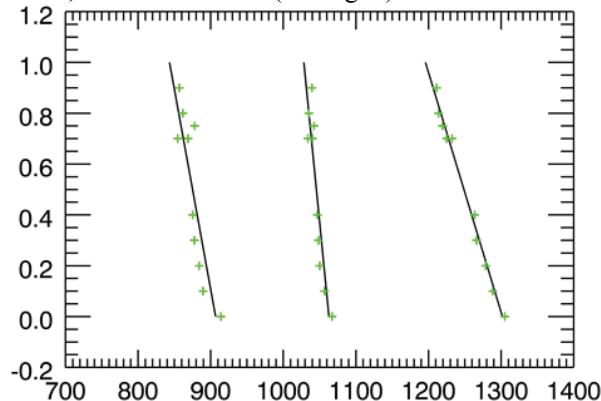


Figure 2. Composition Trend lines from our MGM (suite 2) in Molar % Forsterite vs band center (nm) graph. Spectra with grain size<45 μ m: C1DD[98 (Fo₀), 97 (Fo₁₀), 96 (Fo₂₀), 95 (Fo₃₀), 42 (Fo₄₀), 39 (Fo₇₀), 116 (Fo₇₀), 88 (Fo₇₅), 38 (Fo₈₀), 37 (Fo₉₀)].

Natural olivine samples. We now consider the suite (suite 3) spanning the forsterite-fayalite solid solution series historically considered to derive the olivine composition [1] and apply our MGM approach on its 18 natural samples. The trend line equations established from suite 2 are then used to predict the composition variability based on the minimum deviation from the three trend lines simultaneously. While suite 3 presents an integrated Fo# rms deviation of 14.0, with a 16.9 nm sdt, we find that if one excludes spectra (A,C,E,F,G,P) the resulting suite 4 has an integrated Fo# rms deviation of 4.6 (i.e., comparable to suite 2), with a 12 nm sdt (see Fig. 3). At the exception of P spectrum (Fo₁₈), all other spectra correspond to Mg-rich olivines (Fo#>84), for which our prediction underestimates Fo#. Along with [2, 8], we suspect these spectra are affected by impurities and/or heterogeneities arising from the presence of minor amounts of various cations (Ca²⁺, Mn²⁺, Ca²⁺, Cr²⁺, Fe³⁺, ...).

Though not shown here due to the lack of space, other natural terrestrial and M3 lunar olivine spectra are successfully modeled [7].

Comparison between previous versus current composition trend prediction lines. Compared to previous works, the current M1-1, M2 trend lines present steeper slopes while the M1-2 trend is less steep (Fig. 4). Bandwidths and intensities behave close to [1, 2].

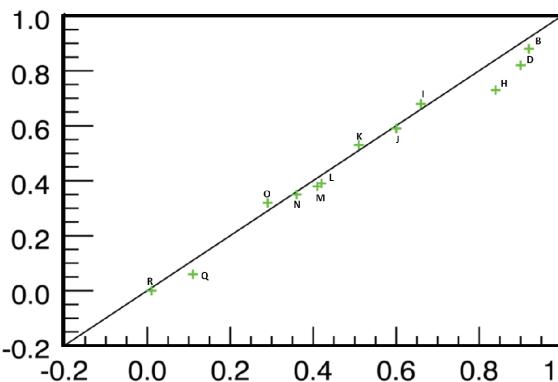


Figure 3. Predicted versus Actual Molar % Forsterite estimates for natural samples (suite 4) from [1], based on our suite 2 (synthetic samples) derived trend lines.

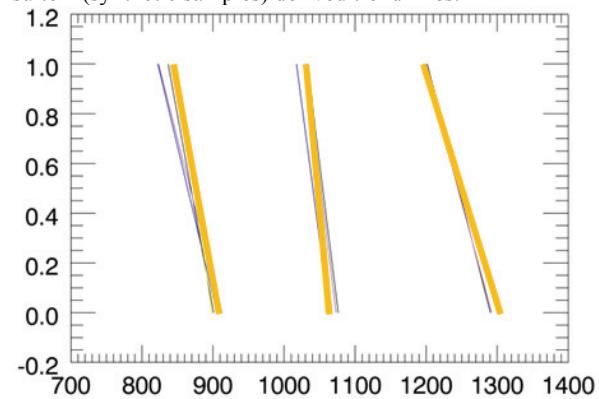


Figure 4. Composition trend lines in Molar % Forsterite versus band center wavelength (nm) graph (in black: ‘Sunshine’ trend lines; in purple: ‘Isaacson’ trend lines from suite 1(Fo range: 0-70) ; in blue: ‘Our’ trend lines from suite1; in thick orange: ‘Our’ current trend lines from suite 2 (Fo range: 0-90)(same as Fig. 2); in yellow: ‘Our’ trend lines from suite 2 without C1DD98 spectrum (Fo#0)).

Conclusions: The trend lines equations derived from the current MGM modeling do not depart very much from previous results. However, the band center positions of the three primary olivine absorptions near 1 μ m (M1-1, M2, M1-2) can be used simultaneously to produce a better constrained prediction across an extended range of olivine solid solution composition either with synthetic or natural samples.

References: [1] Sunshine J. M. and C. M. Pieters (1998) *JGR*, 103, 13,675–13,688. [2] Isaacson P.J. et al (2014) *Am. Miner.*, 99, 467-478. [3] Sunshine J.M. et al. (1990) *JGR*, 95, B5, 6955-6966. [4] Kanner L.C. et al. (2007) *Icarus*, 187, 442-456. [5] Clenet, H. et al. (2011) *Icarus*, 213, 404-422. [6] Clenet, H. et al. (2013) *JGR*, 118, doi:10.1002/Jgre.20112. [7] Pinet P.C. et al. (2018) *LPSC XLIX*, Abstract #1899. [8] Dyar M.D. et al. (2009) *Am. Miner.*, 94, 883-898.