

CONSEQUENCES OF SIGNAL TO NOISE RATIO AND SPECTRAL SAMPLING FOR THE DETERMINATION OF OLIVINE COMPOSITION IN THE INTERMEDIATE INFRARED REGION. S. A. Pérez-López¹, C. H. Kremer^{1,2}, J. F. Mustard¹, M. S. Bramble³, C. M. Pieters¹, and R. O. Green³, ¹Department of Earth, Environmental and Planetary Sciences, Brown University, Providence, RI, ²Department of Geosciences, Stony Brook University, Stony Brook, NY, ³Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA; (sebastian_perez-lopez@brown.edu)

Introduction: Recent studies have established novel applications for the **InterMediate InfraRed** region (IMIR, 4 μm – 8 μm) to analyses of planetary surface composition [1-4]. Among these is the determination of olivine Mg# (molar Mg/[Mg+Fe] \times 100) to $\pm 10\%$ via the position of absorption bands at ~ 5.6 and ~ 6.0 μm which shift systematically with Mg# [1]. Spectral features in the IMIR are less susceptible to space-weathering effects than in the VNIR [4], positioning IMIR as a valuable tool for lunar spectroscopy.

To date, studies of IMIR spectra have used laboratory data, with spectral resolutions and signal-to-noise ratios (SNR) exceeding those expected of remote sensing measurements. The SNR of spectroscopic data acquired from spacecraft decreases due to disturbances from electronic and optical effects inherent to spacecraft observations. Because variations in SNR and sampling rates can affect spectral interpretation by obscuring absorption features at high noise levels and sampling rates [5], here we quantitatively assess the consequences of changing SNR and sampling intervals.

We use a spectral feature fitting routine modeled after Tetracorder [6] to study the effects of artificial degradation on Mg# determination from IMIR olivine spectra. We determine sampling interval and SNR thresholds required for accurate Mg# determination from data equivalent in quality to those anticipated from imaging spectrometers.

Methods: We calculate best-fit matches between artificially degraded olivine spectra of known Mg# and a spectral library of synthetic olivine spectra of known Mg# using a spectral feature fitting routine modeled after Tetracorder [5, 6]. Since both the test spectrum and library spectra are of known Mg#, each round can be considered an Mg# prediction.

Our spectral library consisted of 11 synthetic olivine spectra of known chemistry (SUNY suite) covering the entire Mg-Fe solid solution series at intervals of ~ 10 Mg# [7]. Test spectra consisted of SUNY suite spectra artificially degraded to sampling rates ranging between 10 nm – 80 nm and SNRs ranging between 50 – 200. All spectra were acquired from PDS Geosciences Node Spectral Library, and samples were measured in the Reflectance Experiment Laboratory (RELAB) at Brown University using a Thermo Nexus 870 FTIR spectrometer. In the IMIR region, RELAB acquires reflectance measurements over approximately 650

channels at an average sampling of ~ 6 nm and an SNR of 500, which we estimated by calculating the standard deviation over a flat part of the Mg#70 spectrum.

Test spectra were resampled using the Python *spectres* package [8], which calculates resampled reflectance as a weighted sum of the fraction of reflectance values in the original wavelength domain that fall under the resampled wavelength domain.

To study the effects of variable SNR, we added increasing levels of scaled gaussian noise uniformly across all wavelength bands. We define SNR for a surface of 50% reflectance, where a reflectance level of 0.5 is divided by the standard deviation of the noise spectrum [5].

In the feature fitting routine, first a continuum is removed from both the test spectrum and library spectra. We derive band positions for continuum boundaries from the convex hull of the undegraded SUNY Mg#100 spectra, as high-Mg olivine endmembers had the strongest spectral features in this wavelength range. The resulting continuum bounds were found to be 4.6884 μm and 6.555 μm on the original wavelength domain. In rounds where spectra were resampled, bands nearest 4.6884 μm and 6.555 μm were used. For each spectrum, we found reflectance values associated with the continuum boundaries using a 5-point reflectance average to increase the SNR of those points.

We then adjust the spectral contrast of the library spectra by fitting them to the test spectrum via a linear gain and offset measurement. We calculate an adjusted library spectrum by using an additive constant, k

$$L_1 = \frac{L_0 + k}{1.0 + k}$$

which can be rewritten as the linear equation:

$$L_1 = \frac{k}{1.0 + k} + \frac{1.0}{1.0 + k} L_0$$

and fit with least-squares to find the optimal k value and resulting library spectra [6].

The Root Mean Square Error (RMSE) between the degraded test spectrum and optimized library spectra is then used to evaluate which library spectra provides the best overall fit. If best-fit RMSEs exceeded a threshold of 0.1, they were considered incorrect matches.

Identification rates and associated uncertainties were then calculated for Mg# determination of a given test spectra degraded to various sampling rates and noise levels.

Results: Mg-rich endmembers withstood greater degrees of degradation in both noise and sampling domains, with 100% correct Mg#100 identification persisting through SNRs of 50 and sampling rates of 80 nm (Fig. 1). In more Fe-rich olivines, identification rates ranged from nearly 100% on the least degraded spectra (SNR 200, sampling 10 nm) to <30% on the most degraded spectra (SNR 50, sampling 80 nm) (Fig. 1). Expanding the definition of correct identification to compositions within ± 10 Mg# of the true test spectrum composition significantly broadens the range of viable SNR and sampling rates that result in >90% successful predictions (Fig. 1). We note that correct identification within ± 10 Mg# falls within the uncertainty in Mg# determination initially reported from shifting band positions in laboratory-quality spectra [1].

At a modest SNR expected of CRISM-quality data (SNR = 100 [9]) and 20 nm sampling rate of HOT-BIRD, a novel infrared detector capable of IMIR measurements [10,11], synthetic olivines of all

compositions were identified within ± 10 Mg# in >90% of cases (Fig. 1). This confirms that remote determination of olivine chemistry at spectral qualities expected of imaging spectrometers would be accurate within ± 10 Mg# at 90% confidence levels.

Future Work: Work presented here is limited in scope to studying effects of degradation on pure, synthetic olivine samples. More work is required to expand our understanding of degradational effects on natural olivine samples and olivine mixtures, as well as to model SNRs with radiance observation conditions.

Acknowledgements: RELAB is a multiuser NASA funded planetary science facility. Spectra are available on the PDS Geosciences Node Spectral Library.

References: [1] Kremer et al. (2020) *GRL*, 47 [2] Wilk et al. (2022) *53rd LPSC Abstract #2704* [3] Kremer et al. (2021) *52nd LPSC Abstract #2200* [4] Kremer et al. (2021) *52nd LPSC Abstract #2548* [5] Swayze et al. (2003) *JGR Planets*, 108, E9, 5105 [6] Clark et al. (2003) *JGR Planets*, 108, E12, 5131 [7] Dyar et al. (2009) *American Mineralogist*, 94, 883-898 [8] Carnall (2017) *arXiv: 1705.05165* [9] Murchie et al. (2007) *JGR*, 112, E05S03 [10] Ting et al. (2012) *SPIE* 851104 [11] Cañas et al. (2020) *SPIE* 1150508.

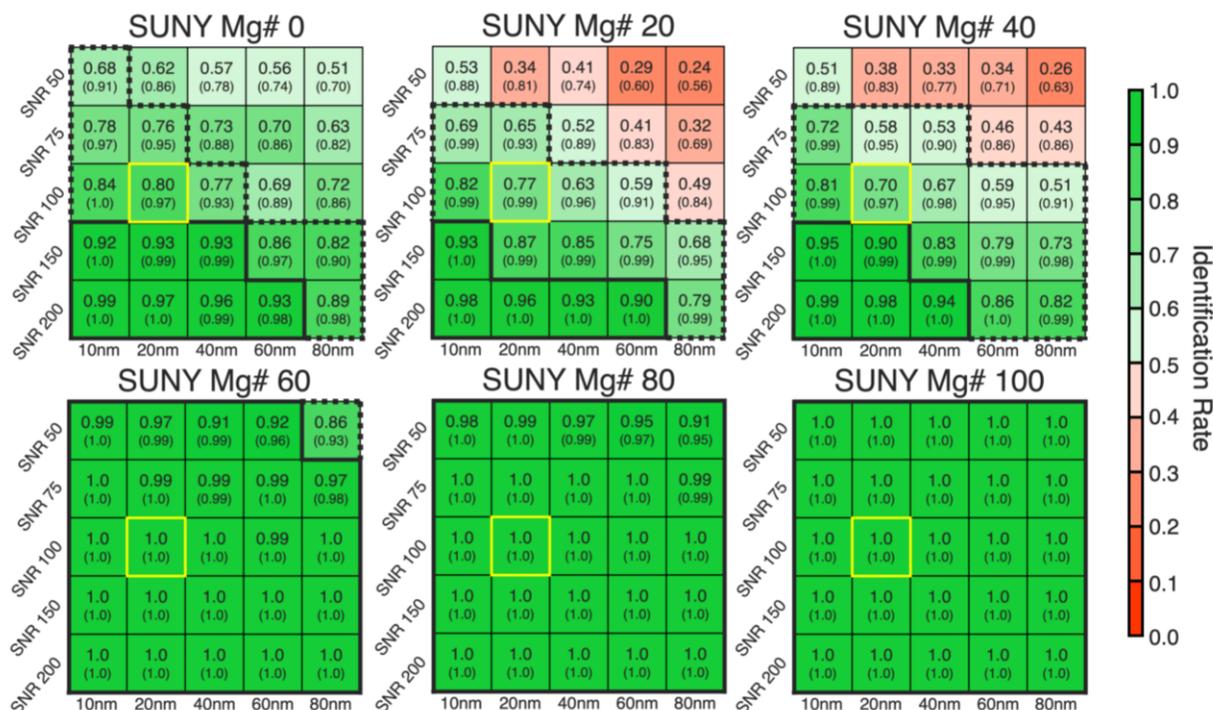


Fig. 1. Results from feature fitting routine on RELAB reflectance spectra of SUNY olivine [1, 7]. Matrices show correct identification rates for a given SNR (rows) and sampling rate (columns), with correct identification rates within ± 10 Mg# written in parentheses. Solid black border denotes parameter space required for >90% correct identification. Dotted black border denotes parameter space required for >90% correct identification within ± 10 Mg#. Yellow outline highlights results for SNR and sampling rate typical of imaging spectrometers. Each grid space represents the results of 400 runs.