

IDENTIFYING AND QUANTIFYING MINERAL ABUNDANCE THROUGH VSWIR MICROIMAGING SPECTROSCOPY: A COMPARISON TO XRD AND SEM. E. K. Leask¹ and B. L. Ehlmann^{1,2}, ¹California Institute of Technology, 1200 E. California Blvd., Pasadena, California, 91125 (eleask@caltech.edu), ²Jet Propulsion Laboratory, 4800 Oak Grove Drive, Pasadena, California, 91109.

Introduction: Visible-shortwave infrared microimaging reflectance spectroscopy is a new technique to identify minerals, quantify abundances, and assess textural relationships at sub-mm scale without destructive sample preparation. Here we used a prototype instrument (Ultra-Compact Imaging Spectrometer, [1]) to image serpentinized igneous rocks and carbonate-rich travertine deposits to evaluate performance relative to traditional techniques: XRD (x-ray diffraction; mineralogical analysis of bulk powders with no texture preservation) and SEM/EDS (scanning electron microscopy/energy dispersive x-ray spectroscopy; analysis of phases and textures using chemical data from polished thin sections). We summarize results discussed further in Leask & Ehlmann (2016) [2].

Methods: Samples from the Samail Ophiolite (Oman) are used as an analog for Martian carbonate and serpentine deposits [e.g., 3] to evaluate the ability of VSWIR microimaging spectroscopy to identify minerals present, distinguish carbonates of different chemistries from minerals with absorptions at similar wavelength positions, and to quantify mineral abundances. Rock samples were measured with UCIS over the wavelength range 0.5-2.5 μm , with 10 nm spectral resolution, and a pixel footprint of 81x81 μm (e.g., Fig. 1). Each sample takes ~3 minutes to image. Subsamples of each rock were sent to external laboratories (ActLabs, K-T Geoservices) for x-ray diffraction (XRD) analyses of powdered samples for mineral identification and quantitative abundance estimates. Two samples were polished, imaged with UCIS, then carbon coated, and imaged on a scanning electron microscope (SEM). Energy-dispersive spectroscopy (EDS) maps were obtained over the area of the sample, providing elemental abundance data for direct comparison with UCIS data.

Linear Unmixing. At this spatial scale, many pixels consist of a single mineral grain. As a first-order approximation, we use linear spectral unmixing [4] to estimate the abundance of phases, assuming most mixed spectra result from areal ‘checkerboard’ mixtures, where endmember spectra combine linearly,

proportional to their areal abundance within a pixel. Endmember selection was refined until average RMS errors were under 0.05.

Mineral Identification: In 13 of 15 samples, UCIS identifies all the same major (>5% abundance) mineral phases as XRD analysis (Fig. 2). Exceptions are a very dark sample (002), where UCIS did not detect 10-19% olivine, and brighter sample (011), where UCIS did not identify ~6% quartz found by XRD. Notably, UCIS data reliably differentiated between carbonate minerals (calcite, dolomite, and magnesite) and serpentine with very similar overall spectra, based on the exact position of the 2.3 μm absorption [5,6] (Fig. 2C). Specific carbonate minerals can be clearly distinguished when each phase extends over several pixels. UCIS also identified spatially coherent rare phases, below the detection limit of powder XRD. Several clasts in conglomerate sample 001 were identified as Al-bearing serpentine or chlorite due to a small 2.25- μm absorption (caused by Al/Mg-OH vibrational overtones [7]). EDS elemental mapping confirms that these clasts contain much more Al than other clasts. Distinctive 0.9- μm pyroxene absorptions [8; Fig 1C, 2B] are seen in samples 001, 007, and 009, though pyroxene is not detected by XRD. Most ‘pyroxene’ spectra show different degrees of partial alteration to serpentine (sharp 1.4- and 2.3- μm hydroxyl absorp-

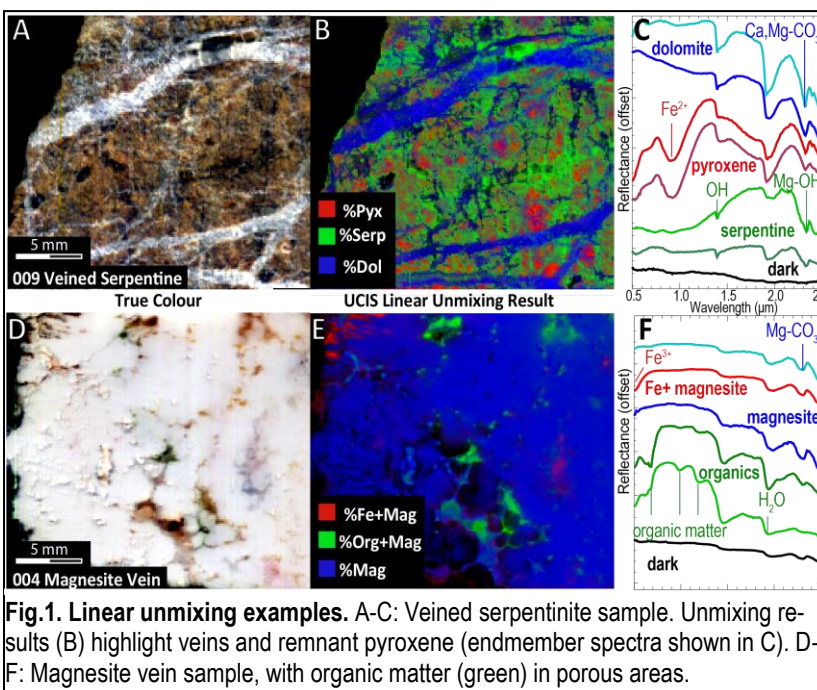


Fig.1. Linear unmixing examples. A-C: Veined serpentinite sample. Unmixing results (B) highlight veins and remnant pyroxene (endmember spectra shown in C). D-F: Magnesite vein sample, with organic matter (green) in porous areas.

tions; Fig. 1C, 1F). These are included in the ‘amorphous’ fraction of XRD results. In magnesite vein samples 004 and 008, absorption features consistent with organic matter are also noted—a sharp ‘red edge’ at ~ 0.8 μm from photosynthetic pigments and minor absorptions in the 1-2 μm range associated with C-H (O), and N-H bonds [9] (Fig. 1F).

Mineral Quantification: Abundance estimates between UCIS and XRD are usually the same within 10-15% (median total difference per sample; see Fig. 2A). Scatter between multiple XRD analyses of different subsamples of the same rock is 5-10%. Given the heterogeneous nature of many of the samples (e.g., 001, 018, 021), natural variance in abundance is expected. For sample 001, areal abundances from EDS and UCIS can be directly compared. Here, determinations are very similar (EDS (UCIS)): 41 (42)% serpentine, 31 (25)% calcite, 21 (18)% mixed carbonate and serpentine, and 7 (14) % pyroxene.

Advantages of this technique: A key advantage of VSWIR microimaging spectroscopy vs. XRD is its ability to obtain mineralogical information with petrographic context, allowing process interpretation. Hence with UCIS, we can get a clearer picture of the bulk mineral composition in altered samples and the processes driving alteration by the ability to simultaneously detect the primary mineral and secondary product. EDS also retains spatial relationships, but requires a high degree of sample preparation, which is expensive and time consuming.

Conclusions: In this study, VSWIR microimaging spectroscopy combined with linear spectral unmixing provides estimates of quantitative mineral abundance consistent with abundance estimates from XRD and EDS. The UCIS prototype instrument demonstrated the ability to identify all VSWIR-active phases and differentiate between carbonate minerals and other minerals like serpentines with major absorptions in the same wavelength region. UCIS is especially well-suited to identify spatially coherent rare phases that would be missed by traditional techniques such as XRD, and tie products to reactants. It is an effective, rapid method to survey a set of samples with minimal preparation.

References:

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