Hyperspectral Imaging of Minerals in the LWIR: Use of Laboratory Reference Measurements for Field Exploitation

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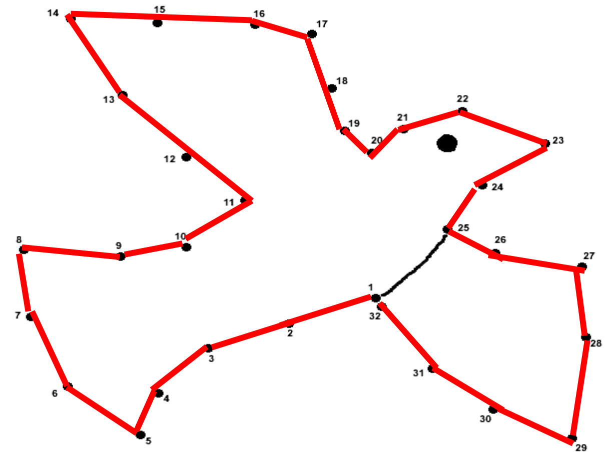
Objectives:

Where are we going with this?

- Can one use <u>laboratory</u> reflectance spectra for HSI field identification in LWIR for solids, e.g. minerals?
- Successful HSI detection of minerals? Both pure and mineral mixtures, by use of the TELOPS Hypercam LW spectrometer with varying solar angle (25°, 35°, and 45° relative to ground), temperature, and diurnal effects?
- Discrimination of the pure and mineral mixtures from one another with the aid of statistical analyses including principal components analysis (PCA), classical least squares (CLS), and multivariate curve resolution (MCR)

Outline

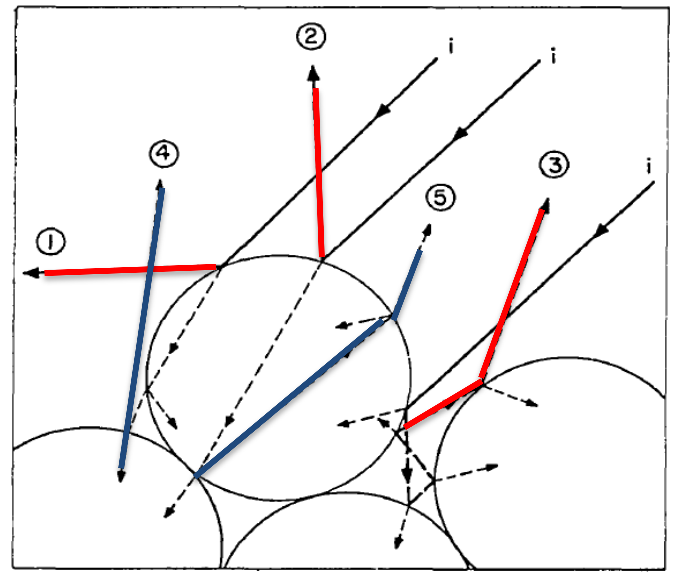
Connecting the dots



- Objectives of Experiment
- Reflectance Spectroscopy
  - Review Some Basics
- Experimental Methods: Laboratory
- Field Experiment Setup
- Results – MCR and other methods

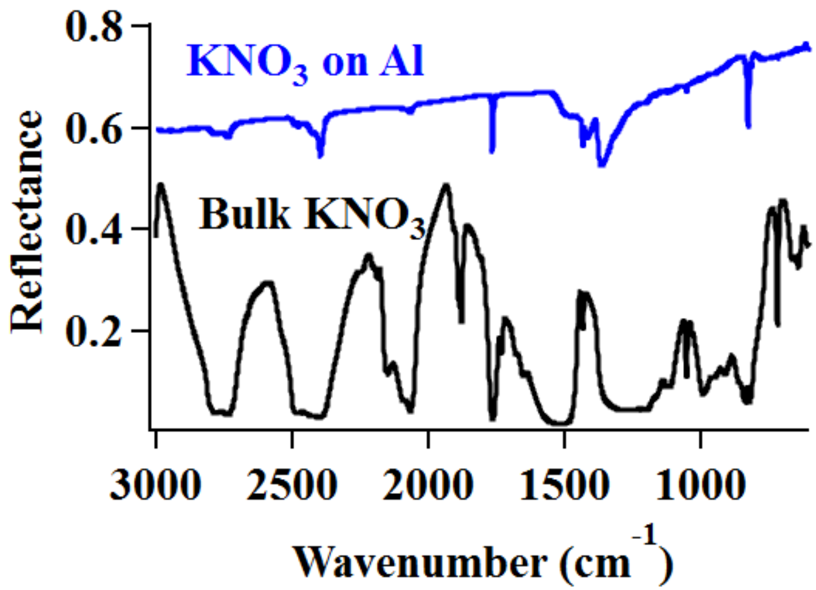
Reflectance Spectra –
Caution: It sometimes gets messy

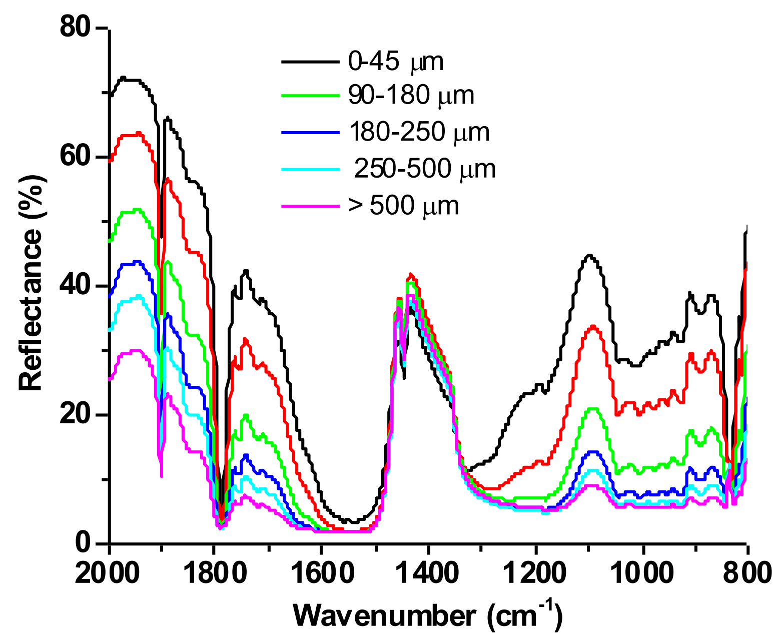
- Reflectance spectra depend on both real and imaginary components (*n*, *k*) of the refractive index as well as particle size and morphology
  - Combination of *surface* scattering and *volume* scattering
    - Surface scattering leads to greater reflectivity, i.e. Reststrahlen features where little energy passes through grain boundaries. Scattering is thus primarily controlled by 1st surface reflections
- Volume scattering generally leads to lower reflectivity – internal absorption, reflection, refraction



Vincent, Robert K., and Graham R. Hunt. "Infrared Reflectance from Mat Surfaces." *Appl. Opt. Applied Optics* 7.1 (1968): 53. Web. 5 Feb. 2016.

Reflection from Solids: Example of morphological effects, sample particle size effects





Measured lab spectra of $NaNO_3$ v. particle size

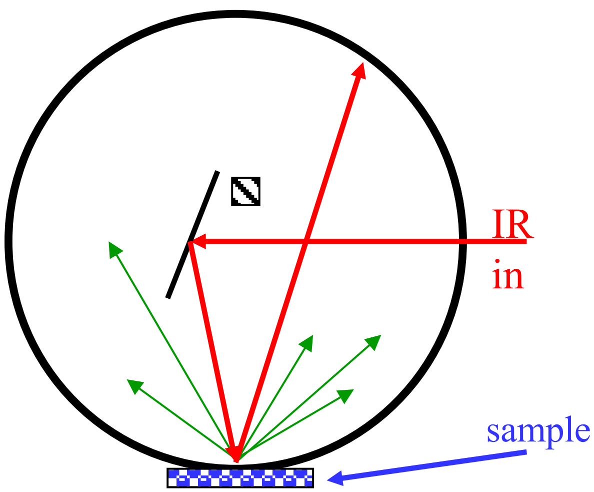
SAME SAMPLE – SPECTRAL VARIATION

Reflectance spectra depend on the <u>sample form and morphology</u>, not always linear in areal coverage or concentration

Laboratory Methods for Spectral Acquisition

Total = specular + diffuse
<u>(also called hemispherical)</u>

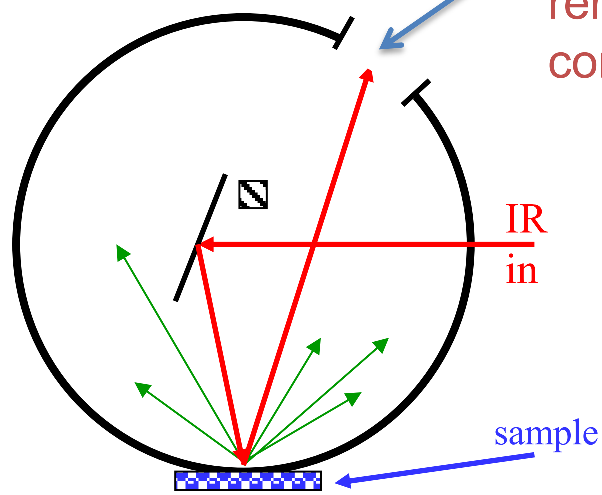
Red = specular
Green = diffuse



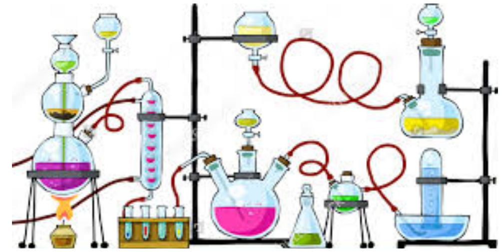
Diffuse only
<u>(removes specular)</u>

Matte gold reference cap is removed for diffuse measurements – removes specular component

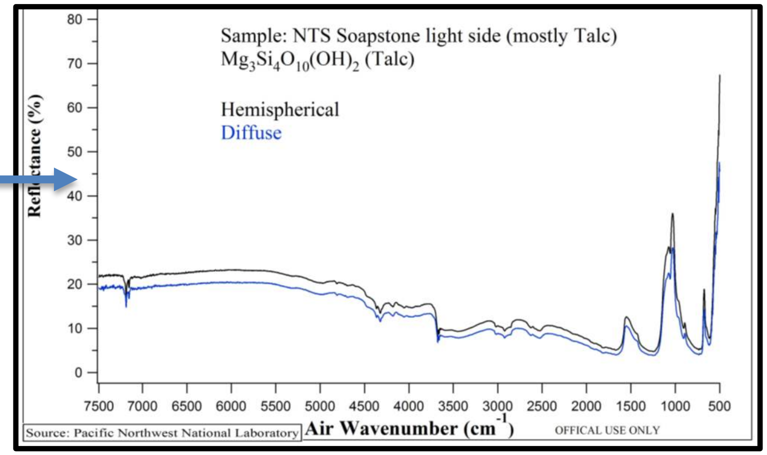
Red = specular
Green = diffuse



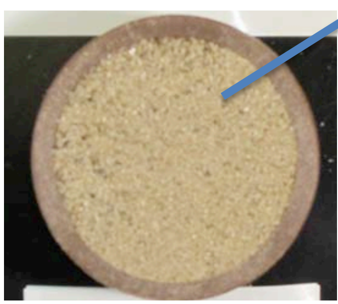
Laboratory Experimental Methods



- Samples: Rocks, polished minerals and powder specimens
- All put at bottom port of 562-G integrating sphere
- Resultant data are hemispherical and diffuse-only spectra

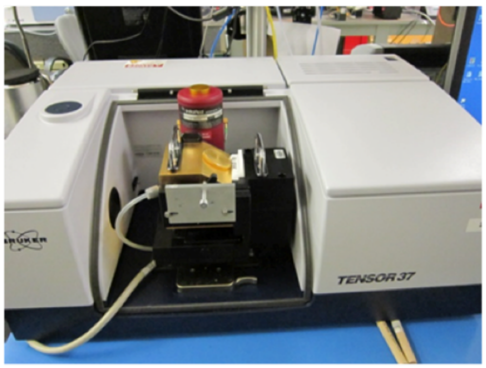


A 562-G integrating sphere



Laboratory Experimental Methods

- Tensor 37 FTIR with an 562-G gold integrating sphere
  - Sample spectrum recorded by tilting the mirror down towards the sample
  - Reference spectrum recorded by tilting mirror up towards matte gold cap

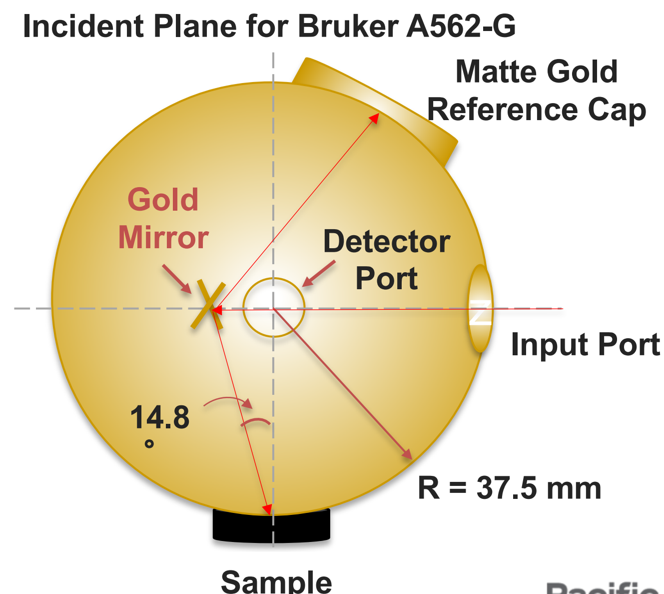


Bruker Optics Tensor 37

Collection Parameters

- 600–6,500 cm^{-1} (1.6 to 16 μm)
- 4 cm^{-1} resolution
- Data point every 1 cm^{-1}

$$\text{Reflectance} = \frac{\text{Sample Spectrum}}{\text{Reference Spectrum}}$$

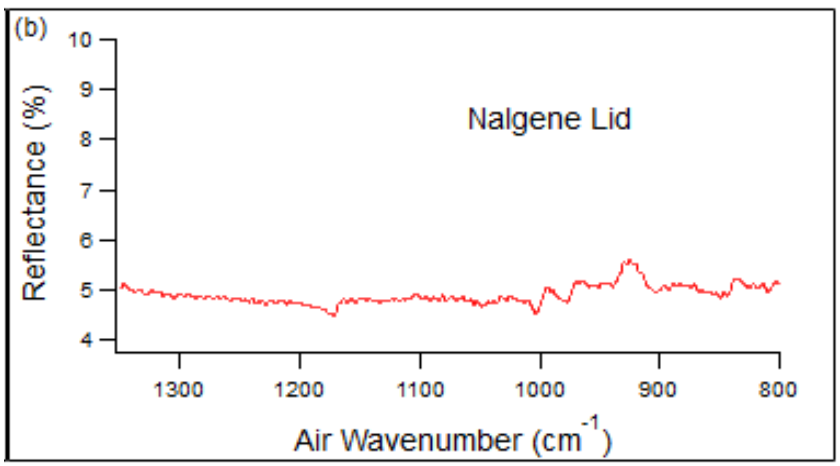


Field Experiment Setup
Telops LWIR Hypercam Sensor

- Field-of-view: 320 x 200 pixels
- Instrument responds in the spectral range of 7.7 to 11.8 μm in the LWIR (1300 - 850 cm^{-1})
- Spectral resolution: 4 cm^{-1}
- Averaged 8 datacubes.
- Sample board distance: 46 ft. (14 m)

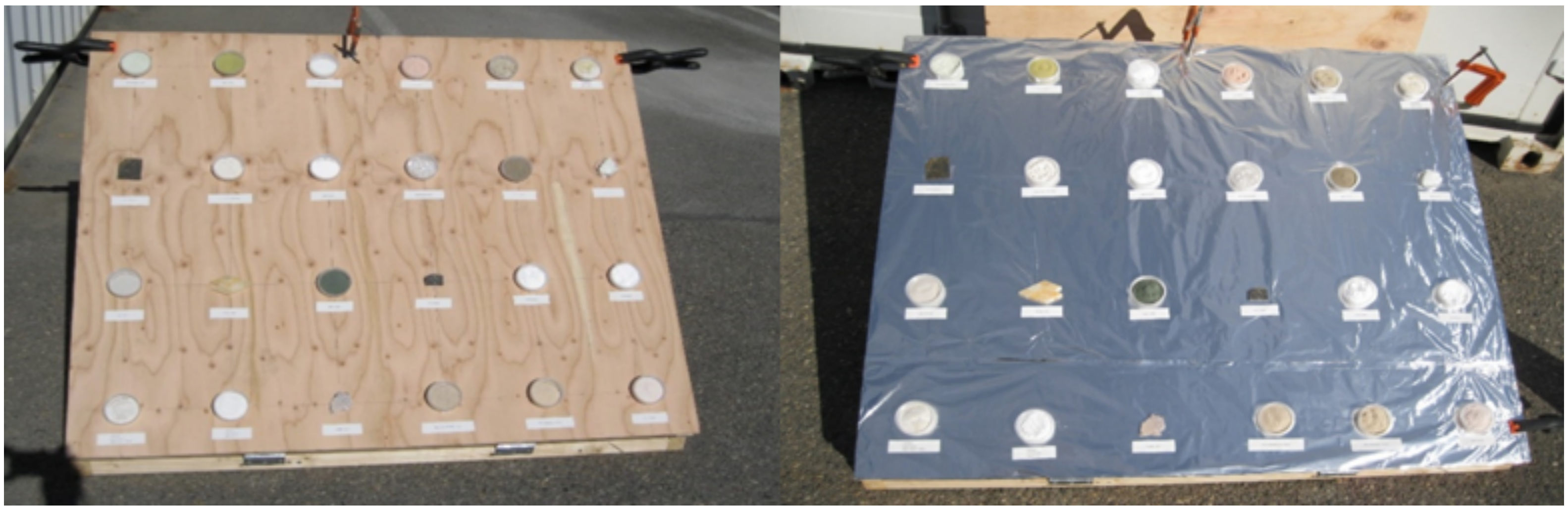
Field Experiment: Samples / Boards

- Samples on board on hinged frame: Wooden dowels cut to create 25°, 35°, 45° ground angles. Plywood boards held on frame w/ C-clamps for easy exchange of sample boards
- Multiple boards: both bare / Al covered
  - 5 samples in rock form – taped directly to wood
  - 19 powders – held in Nalgene bottle lids
- Nalgene lids have very low %R



Field Experiment: Samples Arrangement

- Samples spacing: 8 inch columns, 11.3 inch rows
  - Minerals and powders samples evenly spaced
  - Bare plywood and aluminum foil surfaces

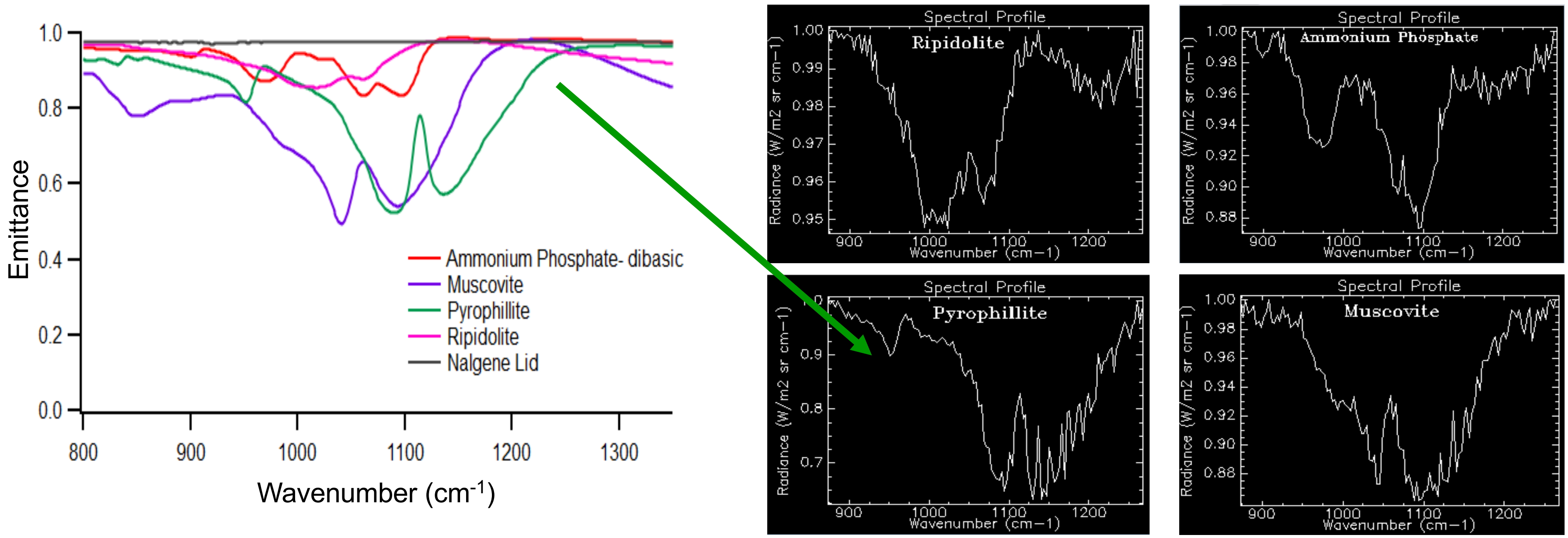


Clinoptilolite	Nontronite	Ammonium Phosphate	Bauxite	Vermiculite	50/25/25 Sodium Carbonate/ Microcline/ Nontronite
Mica Schist (rock)	Dickite	Sodium Carbonate	Muscovite	Quincy Soil	Artinite (rock)
Sand	Faux Onyx (rock)	Ripidolite	Saponite (rock)	Calcium Carbonate	Sodium Phosphate
75/25 Sodium Carbonate/ Sericite	50/50 Caclium Carbonate/ Sand	Pyrophillite (rock)	Sericite	Montmorillonite	Microcline

Field Experiment: ENVI Spectral Profiles

Laboratory Reference Spectra

ENVI Spectral Profiles



- Spectral profiles extracted from single pixels – continuum removed but not corrected for (O_3 and other) atmospheric interferents
- Spectral profiles of Muscovite, Pyrophyllite, Ripidolite, and Ammonium Phosphate had the most defined features in the 850-1300 cm^{-1} region
- Reference spectra of the samples from the laboratory analysis compare well with the spectral profiles from ENVI

Target Detection

- Use a radiance model to set up a target detection strategy
  - Can ‘targeted anomaly detection’ help?
- Use MCR first to examine ‘passive’ end-member extraction
  - Is it even possible? – yes!

Global Models

- Global Model for $CaCO_3$ and Sand
  - Use each target singly (single target detection)
  - Use two iterations
    - Use entire image as clutter (tough detection problem)
    - Remove detections and re-characterize the clutter
  - Use F-test at 99.9% as decision limit
    - Threshold for display, calculate $F_r = F_{stat}/F_{limit}$
    - Pixels with $F_r < 1$ set to 0
    - Pixels with $F_r > 2$ set to 2

Field Experiment: Detection Estimator

Target detection is based on generalized least squares with "clutter suppression." Two iterations were used; detected pixels in the first iteration were removed the suppression in the second iteration.

$$\hat{\mathbf{c}}_k = \mathbf{R}\mathbf{W}_{c,j}^{-1}\mathbf{s}_k\left(\mathbf{s}_k^{\mathrm{T}}\mathbf{W}_{c,j}^{-1}\mathbf{s}_k\right)^{-1}$$

$\hat{\mathbf{c}}_k =$ contributions for target k

$\mathbf{s}_k =$ reflectance spectrum for target k

$\mathbf{R} = M \times N$ matricized image (reflectance)

$\underline{\mathbf{R}} = M_{\mathrm{X}} \times M_{\mathrm{Y}} \times N$ image: $M = M_{\mathrm{X}} \times M_{\mathrm{Y}}$

$\mathbf{W}_{c,1} =$ covariance for the entire image (not centered)

$\mathbf{W}_{c,2} =$ covariance for the entire image w/o detected pixels from first iteration (not centered)

The matricized image corresponds to the estimated reflectance given by

$$\mathbf{r}_m = \left(\mathbf{x}_m - \mathbf{b}\right)\mathrm{dg}\left(\mathbf{x}_0 - \mathbf{b}\right)^{-1}$$

$m = 1,\ldots,M$

$\mathbf{r} =$ row of $\mathbf{R}$ as a column vector

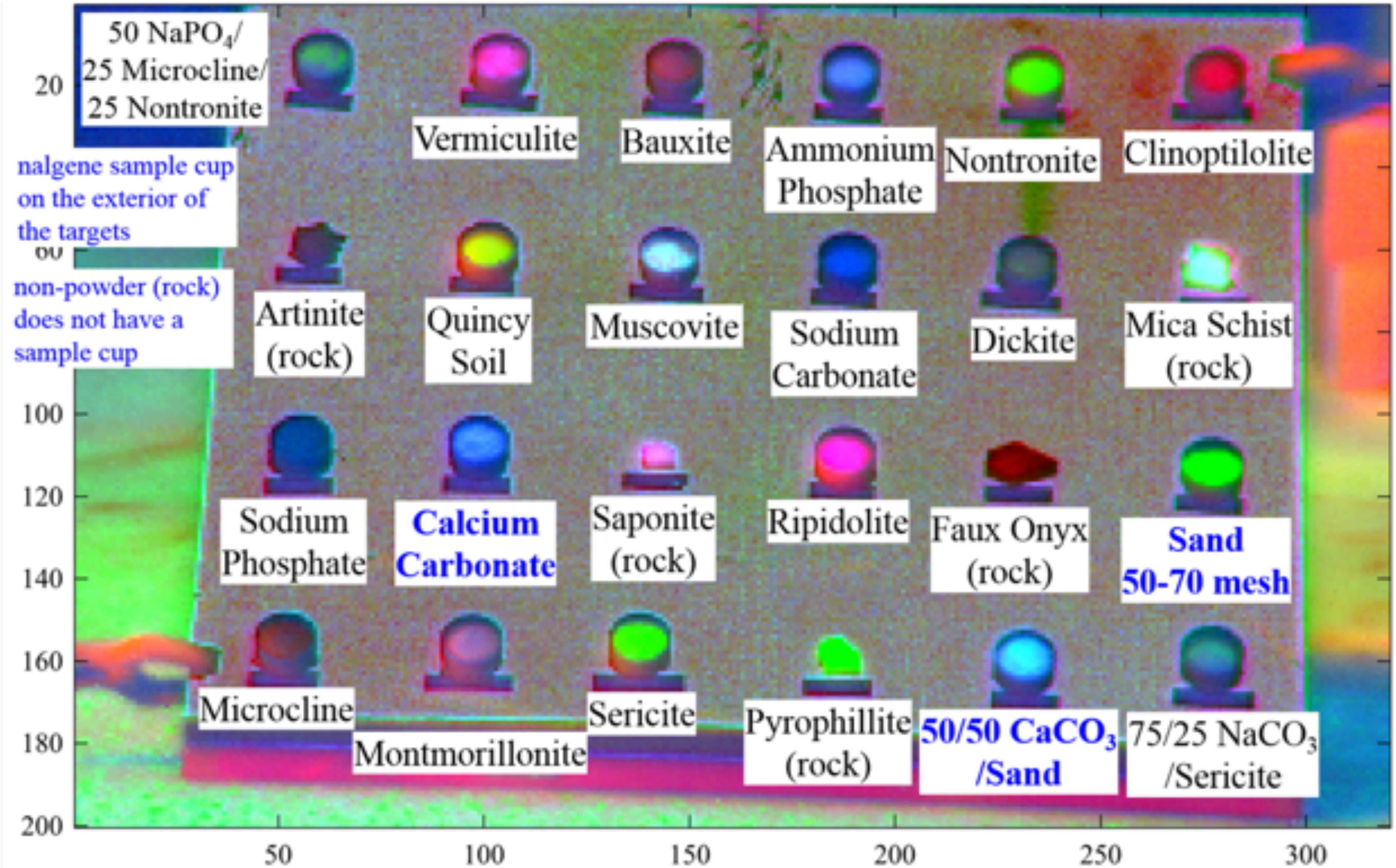
$\mathbf{x} =$ measured radiance

$\mathbf{b} =$ black body radiance

$\mathbf{x}_0 =$ sky radiance

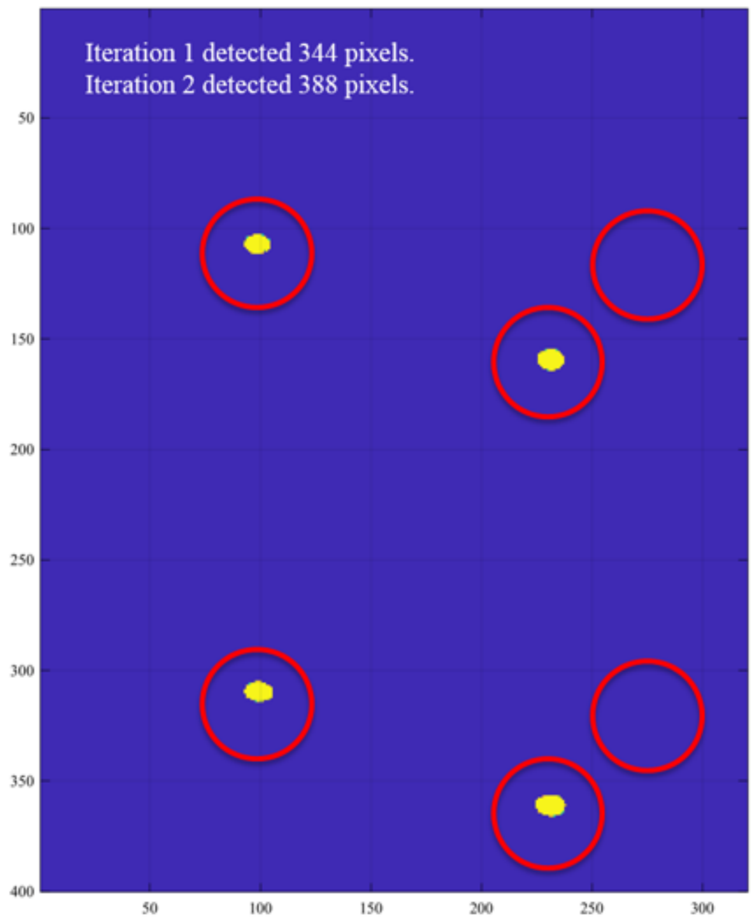
$\mathrm{dg}\left(\mathbf{x}\right)$ creates a diagonal matrix

Graphical Representation Based on PC Scores

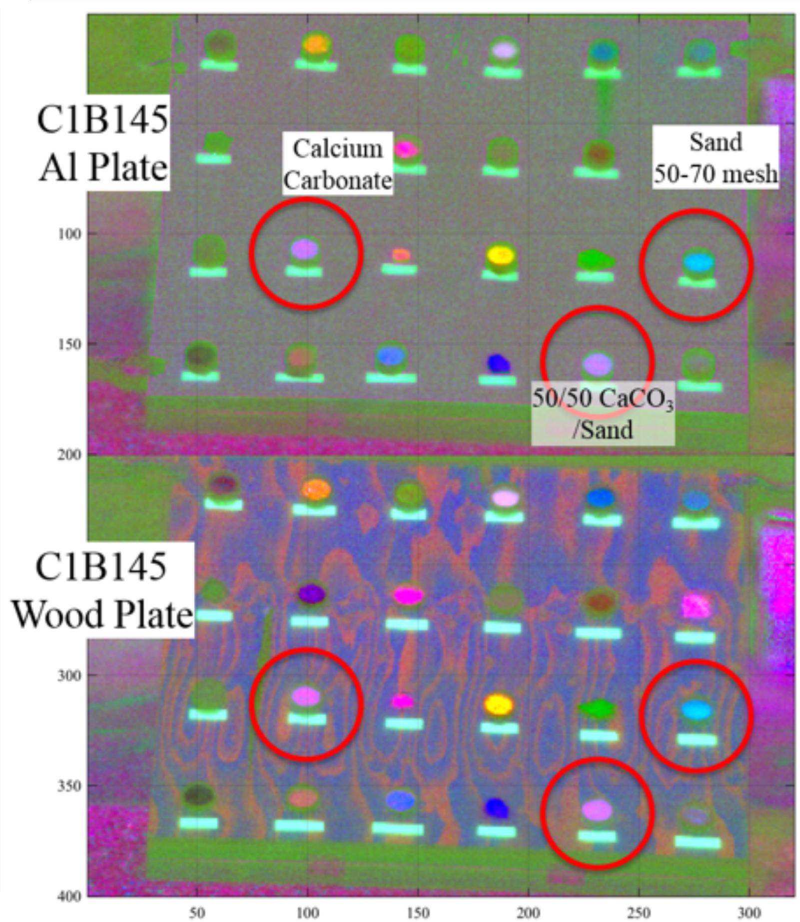


Field Experiment: Detection of Calcite ($CaCO_3$)

Target detection results for $CaCO_3$: Iteration 2



Scores image (auto-contrasted) for visualization



Only $CaCO_3$ is detected (including the 50/50 mixture)!

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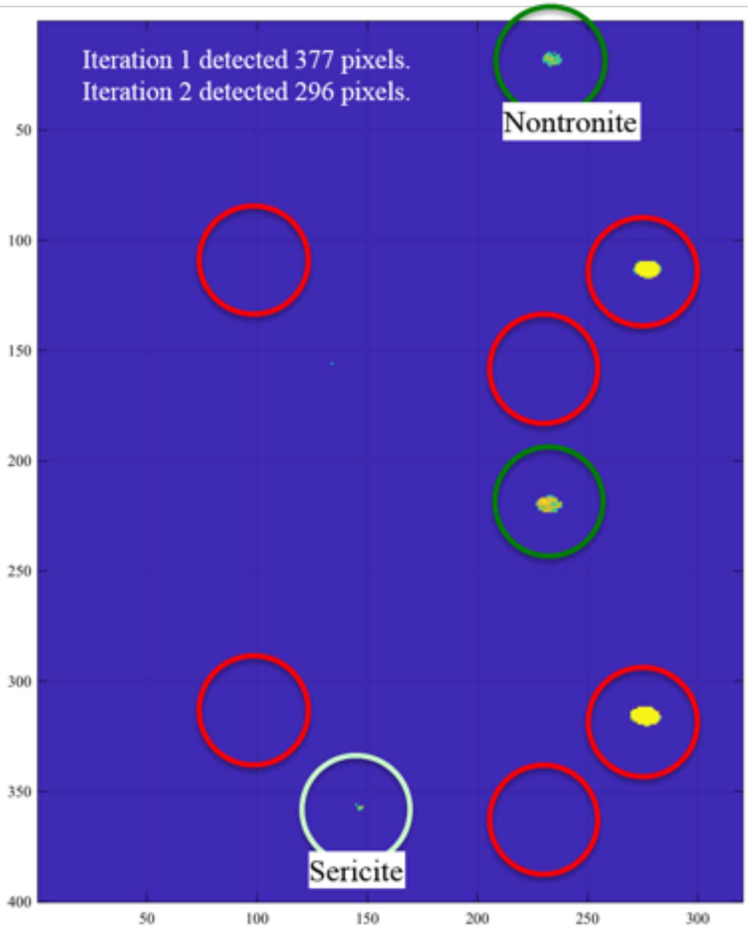
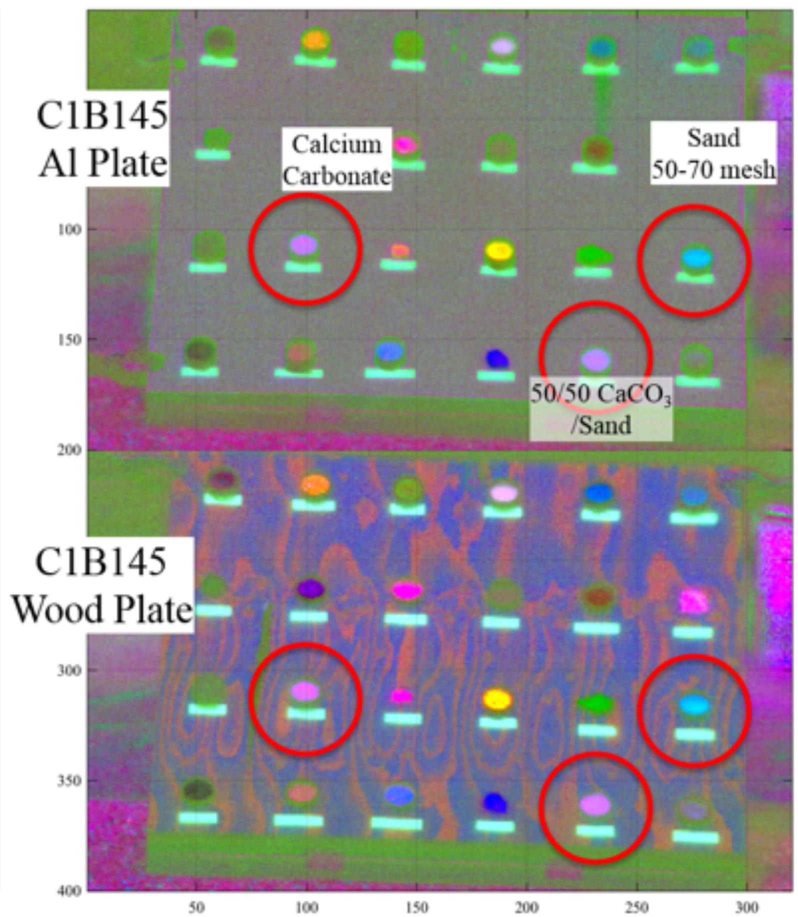
Field Experiment: Detection of Sand (SiO_2)

Target detection results for Sand: Iteration 2



Scores image (auto-contrasted) for visualization

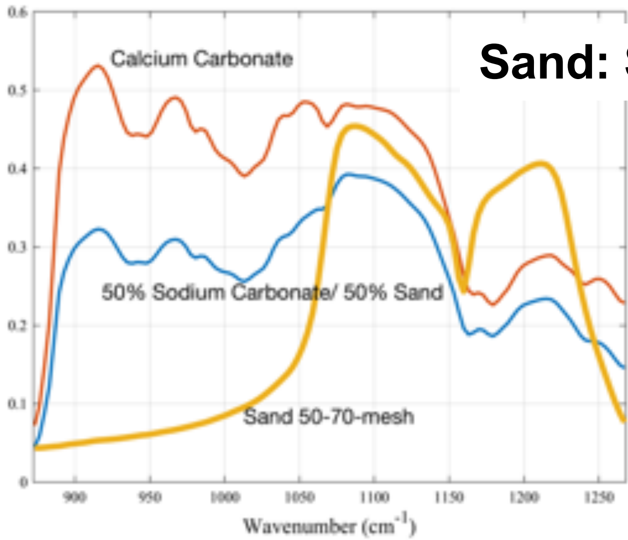


Sand is detected (none in the 50/50 mixture). Nontronite is a false alarm. Sericite has a minor false alarm on the wood plate.

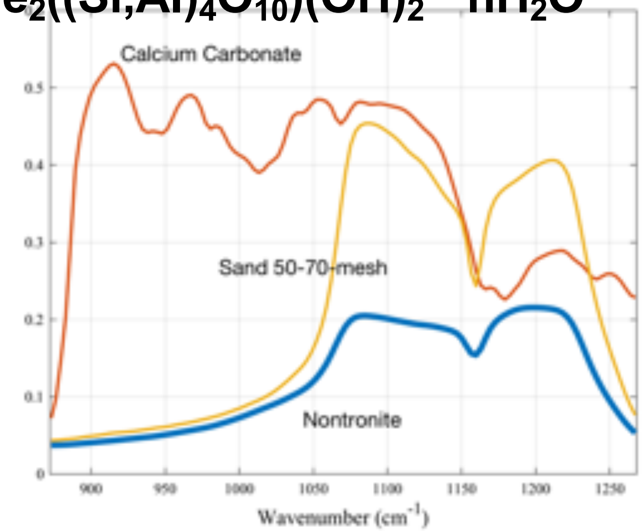
Spectral Analysis of Detected Species: Compare Laboratory Measurements

50/50 mixture looks like $CaCO_3$ at lower concentration

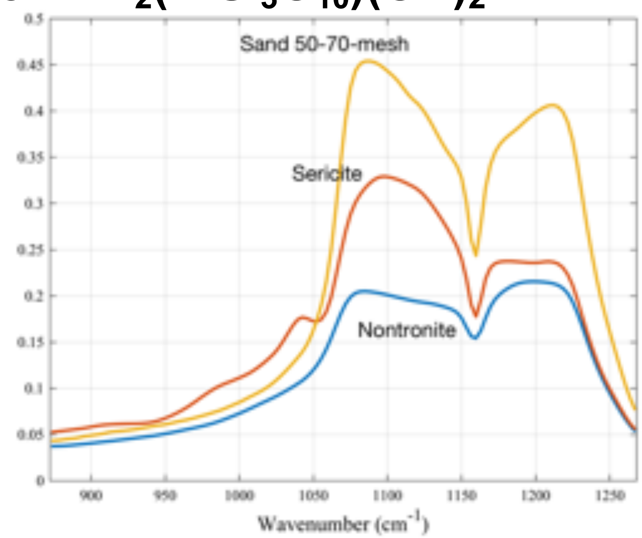
Sand: SiO_2



Nontronite: $Na_{0.3}Fe_2((Si,Al)_4O_{10})(OH)_2 \cdot nH_2O$



Sericite: $KAl_2(AlSi_3O_{10})(OH)_2$



Nontronite looks like “low concentration” Sand

Sericite is ~similar to Sand

Sericite and Nontronite both have high silica content

Summary & Future Work

- Laboratory reflectance spectra can be used for similar samples (same morphology).
  - Particle size can vary for real-world applications
  - Need library that has morphological effects (or model using *n*,*k*)
- We will continue to develop and compare various exploitation algorithms for such minerals.

Acknowledgments

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