UNIVERSITY OF TWENTE.

INFRARED SPECTROSCOPY ON MINERALS AND ROCKS

CHRIS HECKER (ITC)

JULY 2013

ITC

FACULTY OF GEO-INFORMATION SCIENCE AND EARTH OBSERVATION

INTRO: CHRIS HECKER

- **CV**
  - **B.Sc. Earth Sciences (1996)**
  - **M.Sc. Earth Sciences (1999)**
  - **University of Basel, Switzerland**
  - **PhD Thermal RS (2012) ITC**

- **Lecturer Geologic Remote Sensing (70%)**
- **Researcher Geologic Remote Sensing (30%)**

- **Areas of interest:**
  - **Geologic RS**
  - **Thermal RS**
  - **Imaging Spectrometry**

- **Email: c.a.hecker@utwente.nl**

INTRO UT-ITC (IN A NUTSHELL)

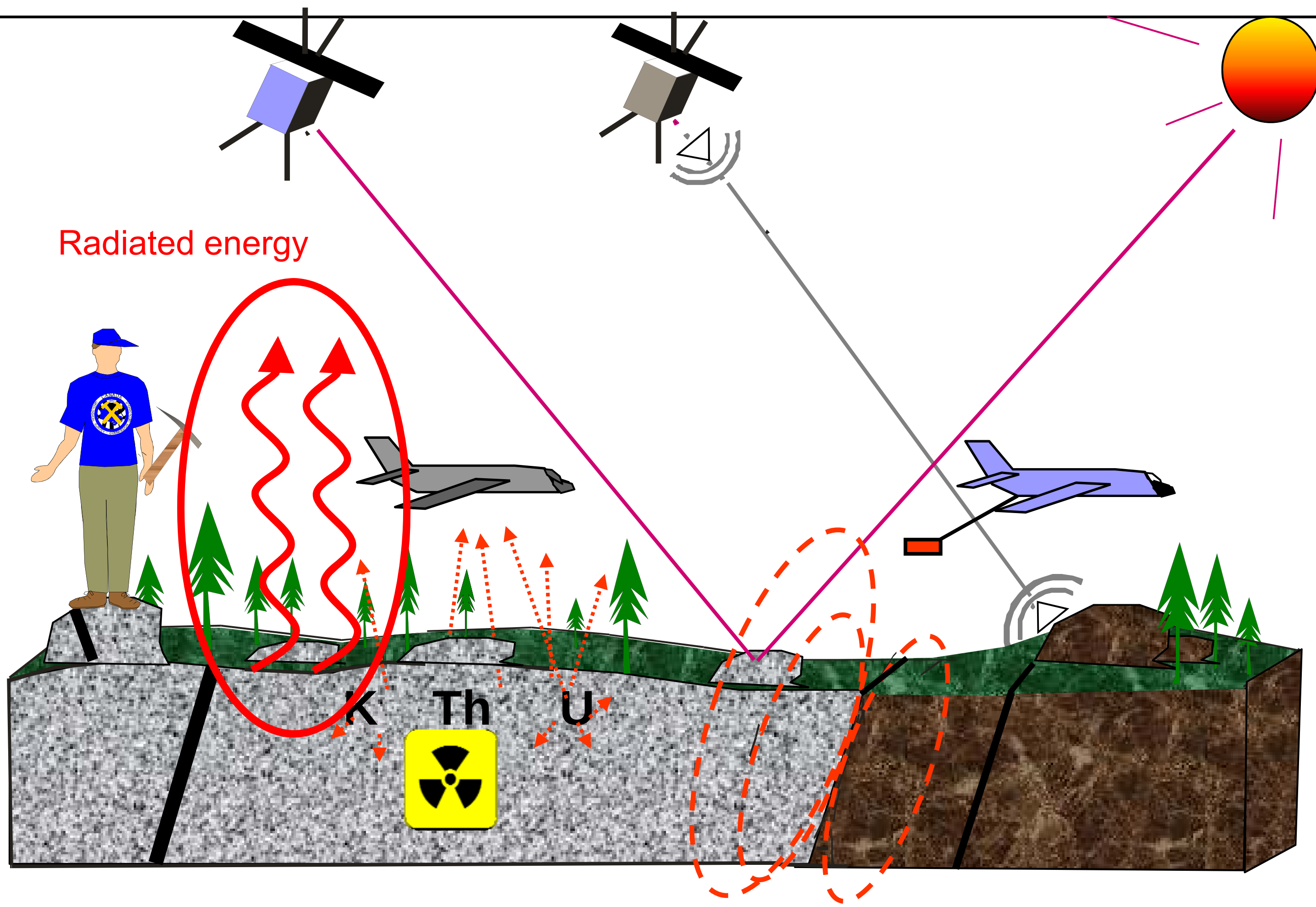
- Mission:
  development and transfer of knowledge in geo-information science and earth observation
- Academic level:
  PhD/MSc/Master/Postgraduate Diploma
- Target group:
  young and mid-career professionals, and scientists from developing and emerging countries, increasingly professionals from industrialised countries
- Framework
  international development cooperation

OUTLINE OF LECTURE

- ***SWIR vs TIR***
- Emissivity spectra of Minerals and Rocks
- Ground-based setups
  - Laboratory
  - Field
- Mapping methods
- Case study: TIR+PLSR

THERMAL INFRARED

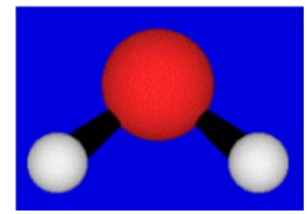
ONE OF THE TOOLS IN THE MODERN EARTH SCIENTIST'S TOOLBOX



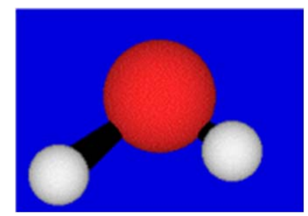
FUNDAMENTAL VIBRATIONAL FREQUENCIES

- The bonds in a molecule or crystal lattice are like springs with attached weights: the whole system can vibrate
- Different types of vibration possible
- Each have different Energy levels
- Combination of absorption features can be diagnostic
- Examples:
  - Al-OH, 2.20 µm
  - Mg-OH, 2.3 µm
  - $Ca\text{-}CO_3$, 2.32-2.35 µm
  - Si-O, ~ 9-10 µm

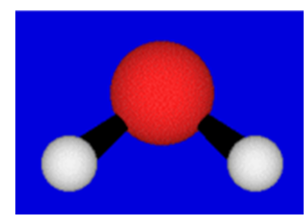
Stretching



Asymetric Stretching

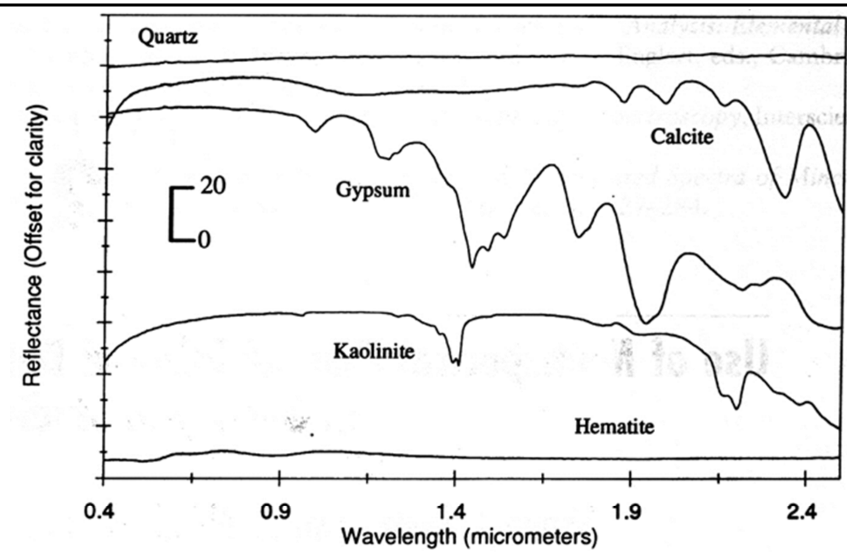


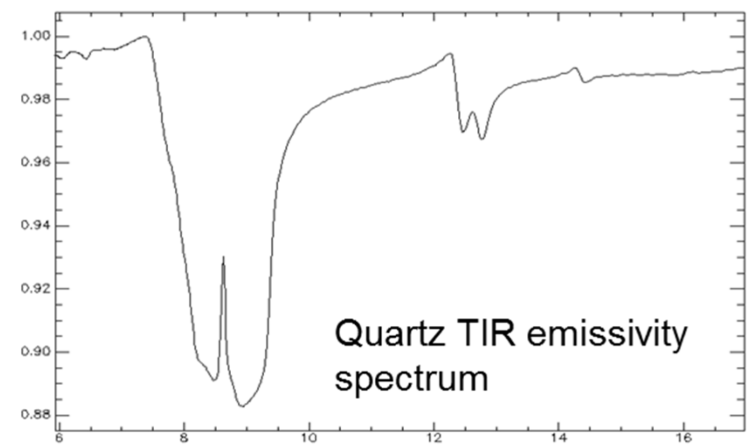
Bending



WHY EMISSIVITY SPECTRA?

- VIS-SWIR features in minerals with:
  - Iron
  - Hydroxyl / water
  - Sulfates
  - Carbonates
  - Phosphates
- No SWIR features for non OH-bearing Silicates => TIR emissivity spectra needed





Rule of Thumb:
- VNIR/SWIR shows alteration products
- TIR shows differences in rock composition

OUTLINE OF LECTURE

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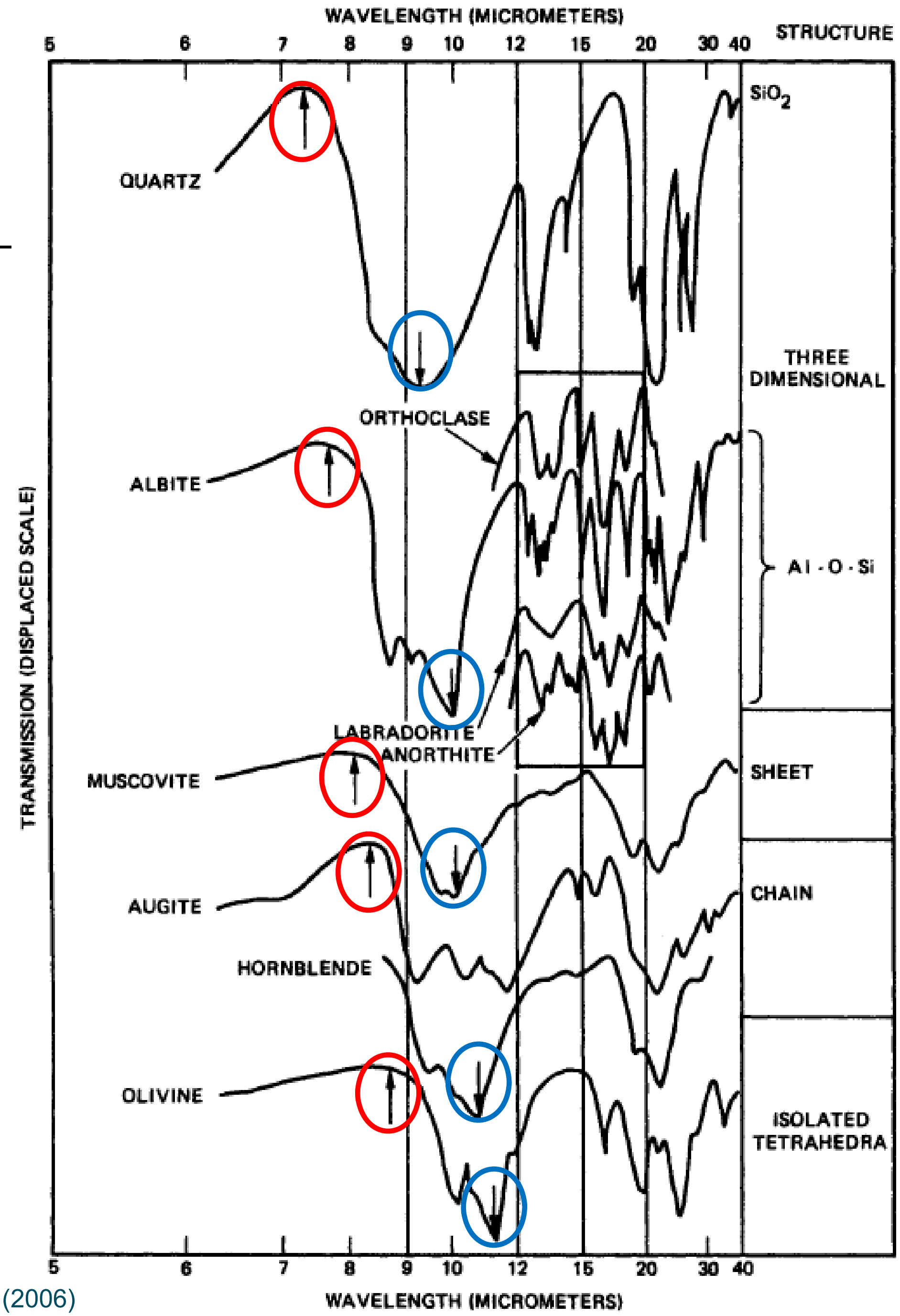
TYPICAL MINERAL SPECTRA

- Reststrahlen feature
  - Strong reflection peak / emission minimum due to fast change in refractive index and center of strong absorption band.
  - Causes emissivity low
  - Shape is diagnostic for silicates and other minerals

- Christiansen frequency
  - Wavelengths where refractive index is close to unity => little scattering
  - If not in absorption band, causes high transmission and low reflectance
  - Visible as emissivity maxima in spectra

TYPICAL MINERAL SPECTRA (CONT'D)

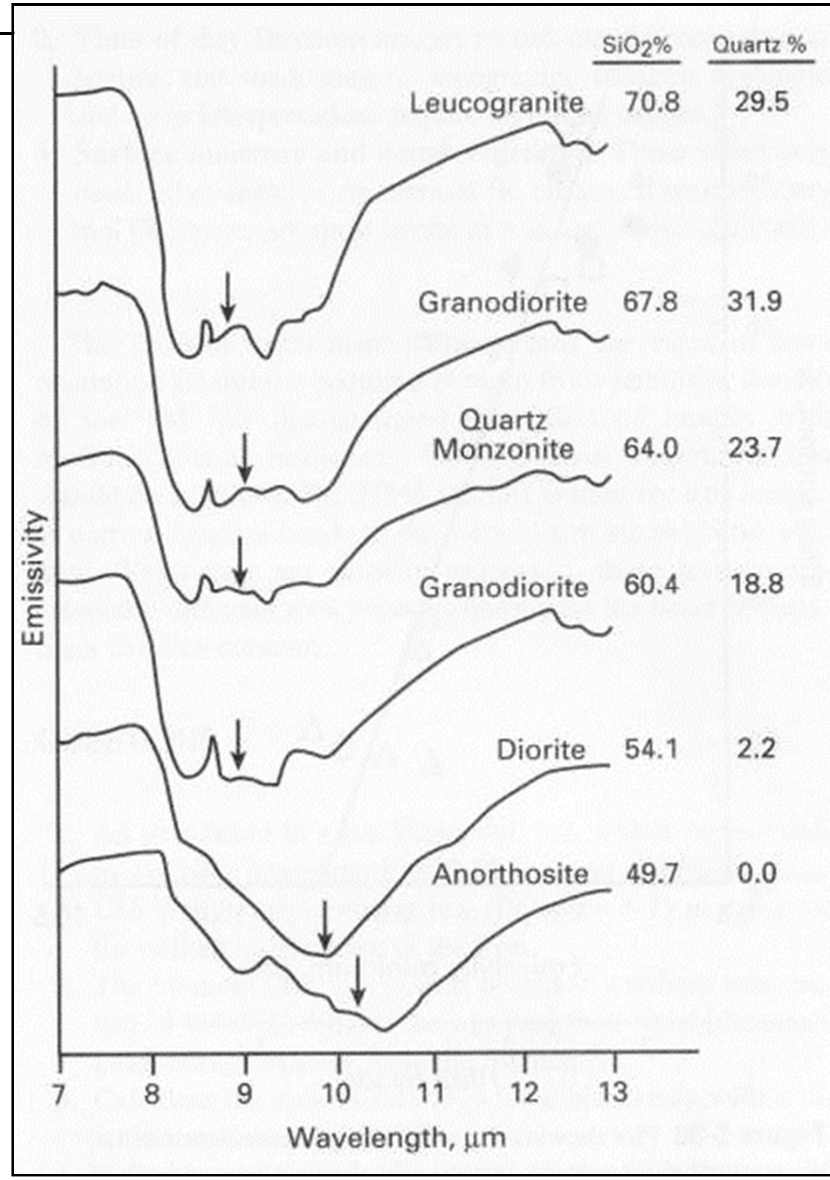
- Mineral (transmission) spectra showing:
  - Christiansen features (up arrows)
  - Reststrahlen features (down arrows)
  - Positions shift to longer wavelengths with decreasing Si-O_4 tetrahedra polymerization.



Source: Elachi and van Zyl (2006)

TYPICAL ROCK SPECTRA

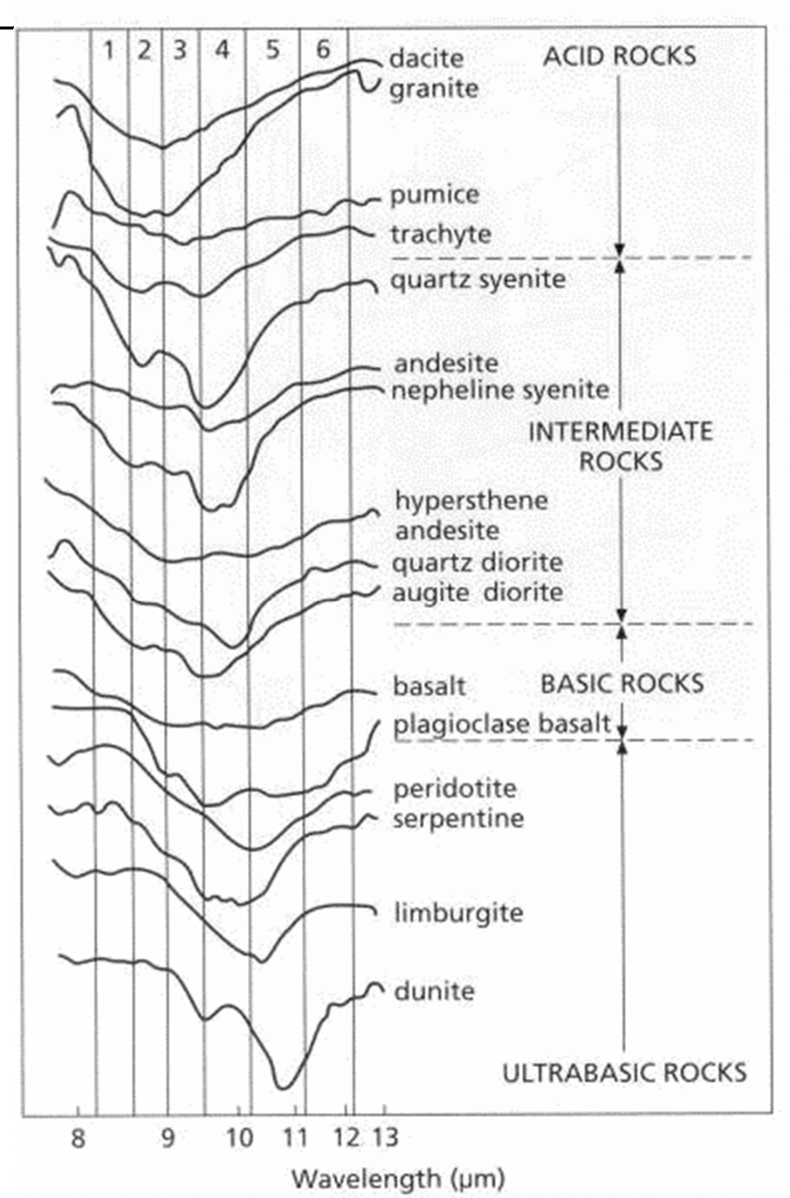
- Rock spectra usually more complex than mineral spectra
- Rock spectra combine features of their main mineralogy
- Acidic rocks show reststrahlenband at lower wavelength than basic rocks
- Change in emissivity minimum can be used for mapping igneous rocks of variable SiO2 content



- Source: Sabins (1997)

TYPICAL ROCK SPECTRA (CONT'D)

- Multi-band thermal systems can help distinguish different rock types and compositions
- Vertical lines and numbers indicate 6 bands of the Thermal Infrared Multispectral Scanner (TIMS)



- Source: Drury (2001)

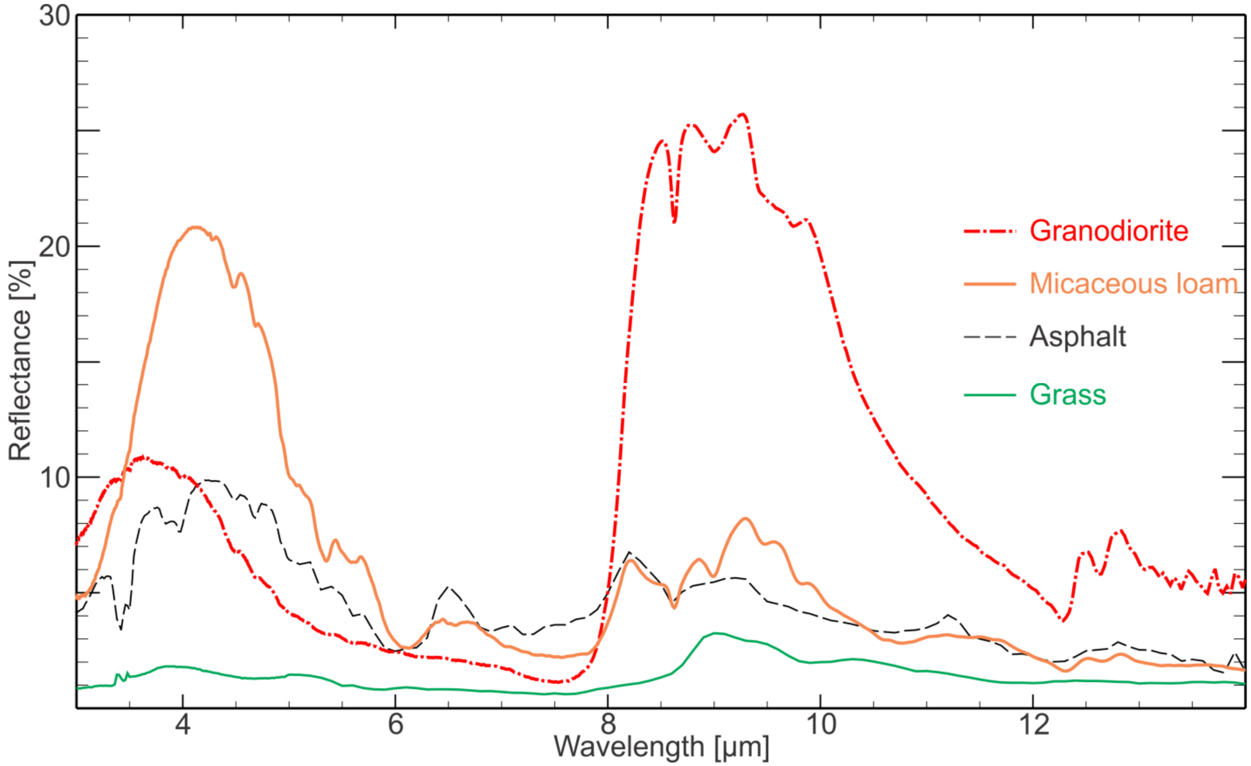
TYPICAL ROCK SPECTRA (CONT'D)

What can we do with it in rock / soil mapping?

- Christiansen frequency
  - Exact position not diagnostic in mixtures
  - Generally high emissivity around 7.5 μm (and 12 μm) useful in TεS.
- Reststrahlen feature
  - General position / shape can give hint in multispectral mapping (e.g., silica%).
  - "Deciphering" of reststrahlen feature used for quantitative analysis in spectroscopy (e.g., PLSR or unmix)
  - Reststrahlen feature of rocks are great for practicing field spectroscopy (before attempting e.g., plants)

TYPICAL ROCK SPECTRA (CONT'D)

- Spectral contrast of rocks much higher than in soils or vegetation
- Example of DHR spectra from ASTER speclib



Source: Hecker et al (2013) Thermal Infrared Spectroscopy in the Laboratory and Field in Support of Land Surface Remote Sensing, in “Thermal Infrared Remote Sensing”, Springer.

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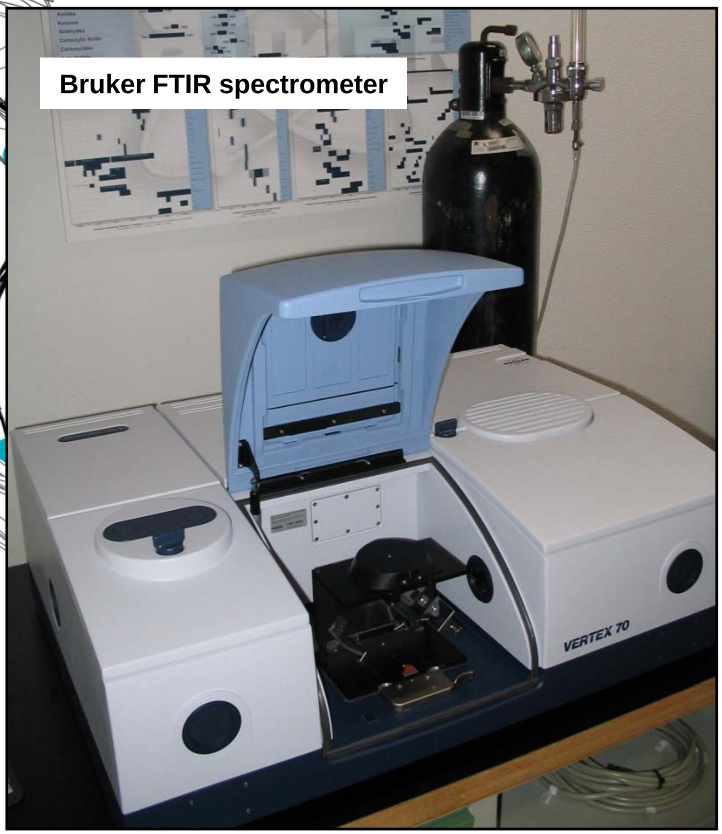
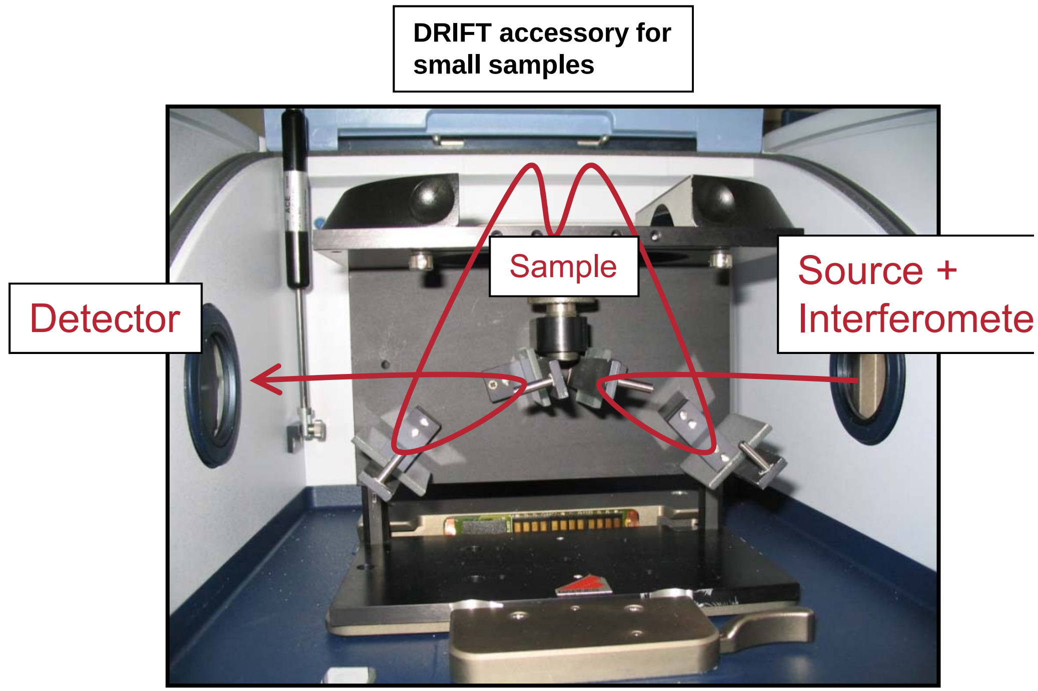
THE SPEC LAB FAMILY PORTRAIT

LABORATORY FTIR BRUKER & DRIFT



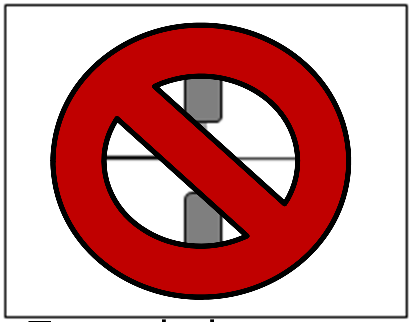


TYPICAL LAB SPECTROMETER WITH DIFFUSE REFLECTANCE (DRIFT) SETUP

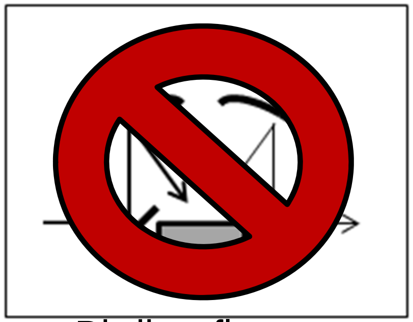
LABORATORY – SAMPLE CONSIDERATIONS

-Designed for small powder samples
-Sampling spot and space too small for most geologic samples

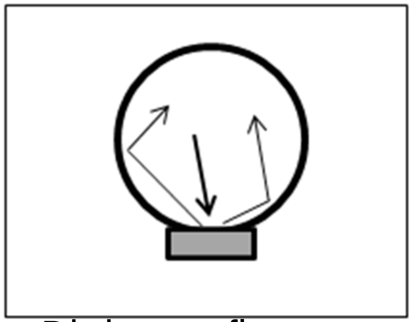
LABORATORY – GEOMETRY CONSIDERATIONS



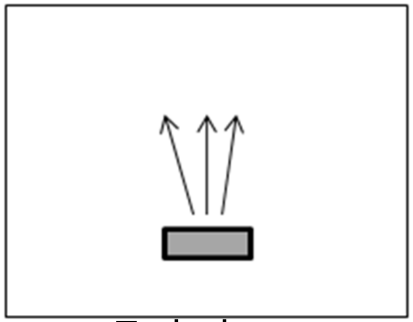
Transmission



Bi-dir refl



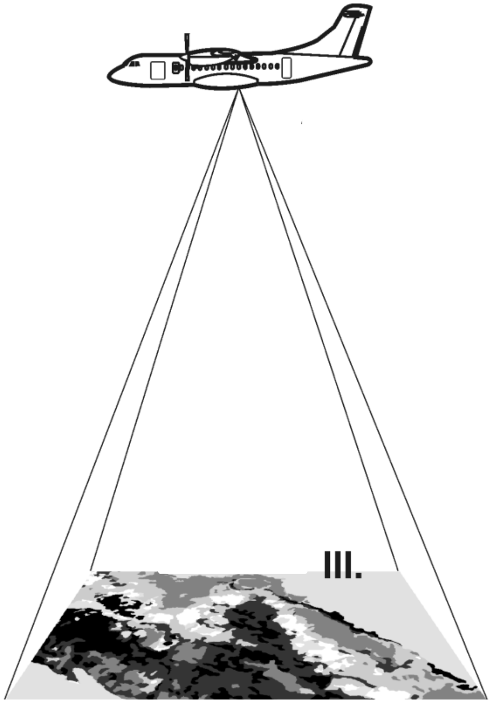
Dir-hem refl



Emission

Quantitative comparison with RS data: DHR or Emission only

Emission: careful temperature control of sample needed



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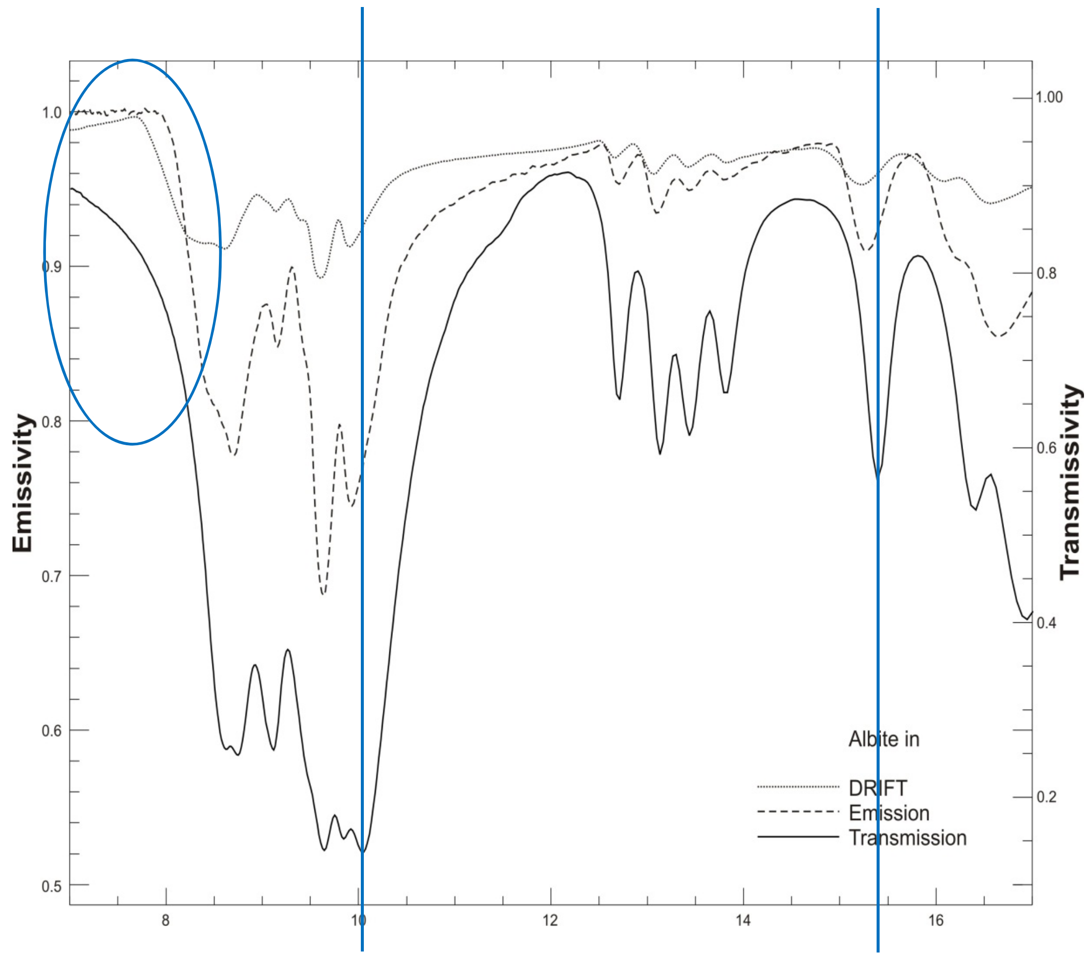
Source: Hecker et al (2010); van Ruitenbeek (2007)

LABORATORY – GEOMETRY CONSIDERATIONS (CONT'D)

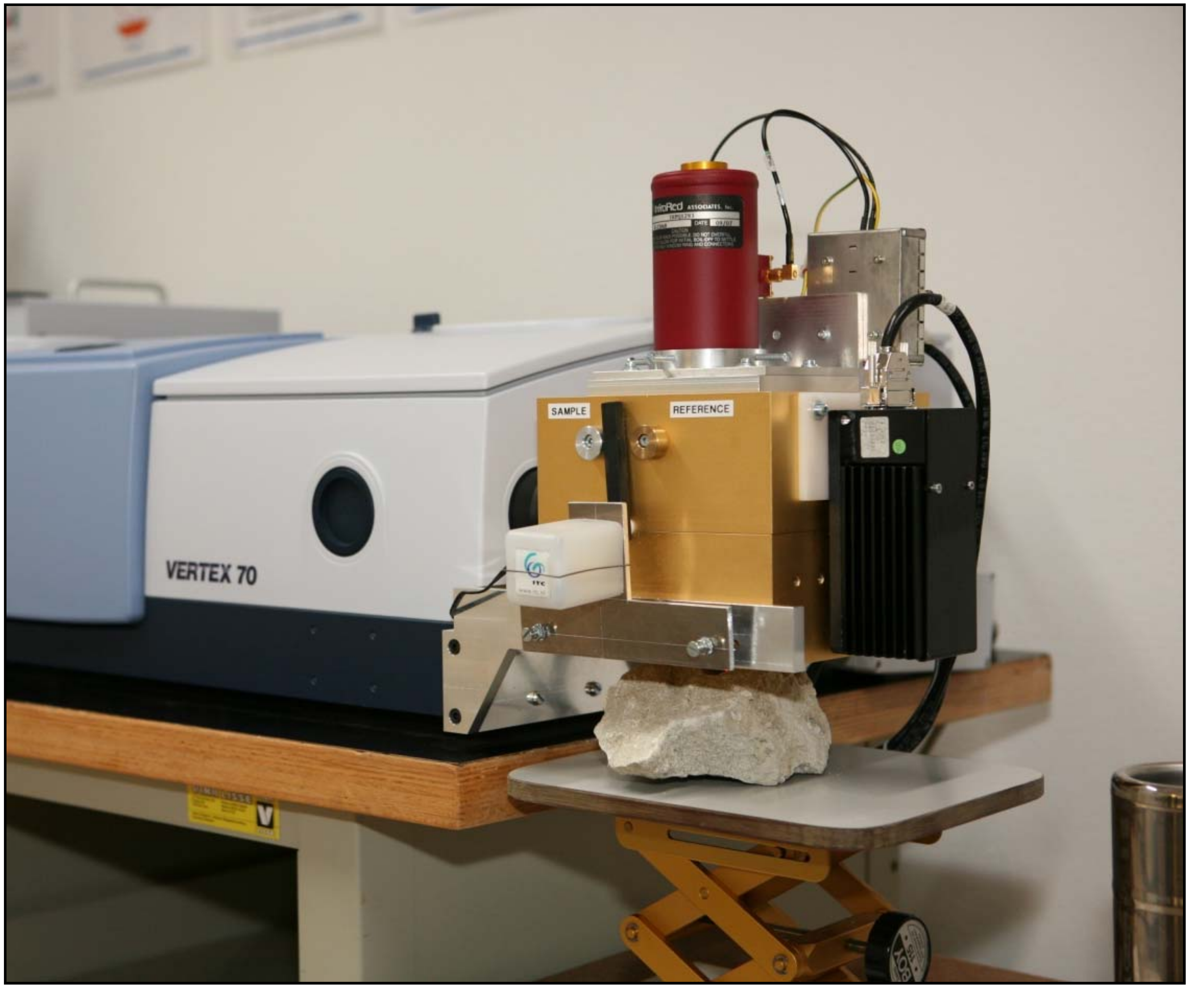
- Same Albite sample
- Measured with DRIFT, DHR, transmission.
- Qualitatively similar
- Quantitatively different (wavelength shifts, relative feature depths … etc.)



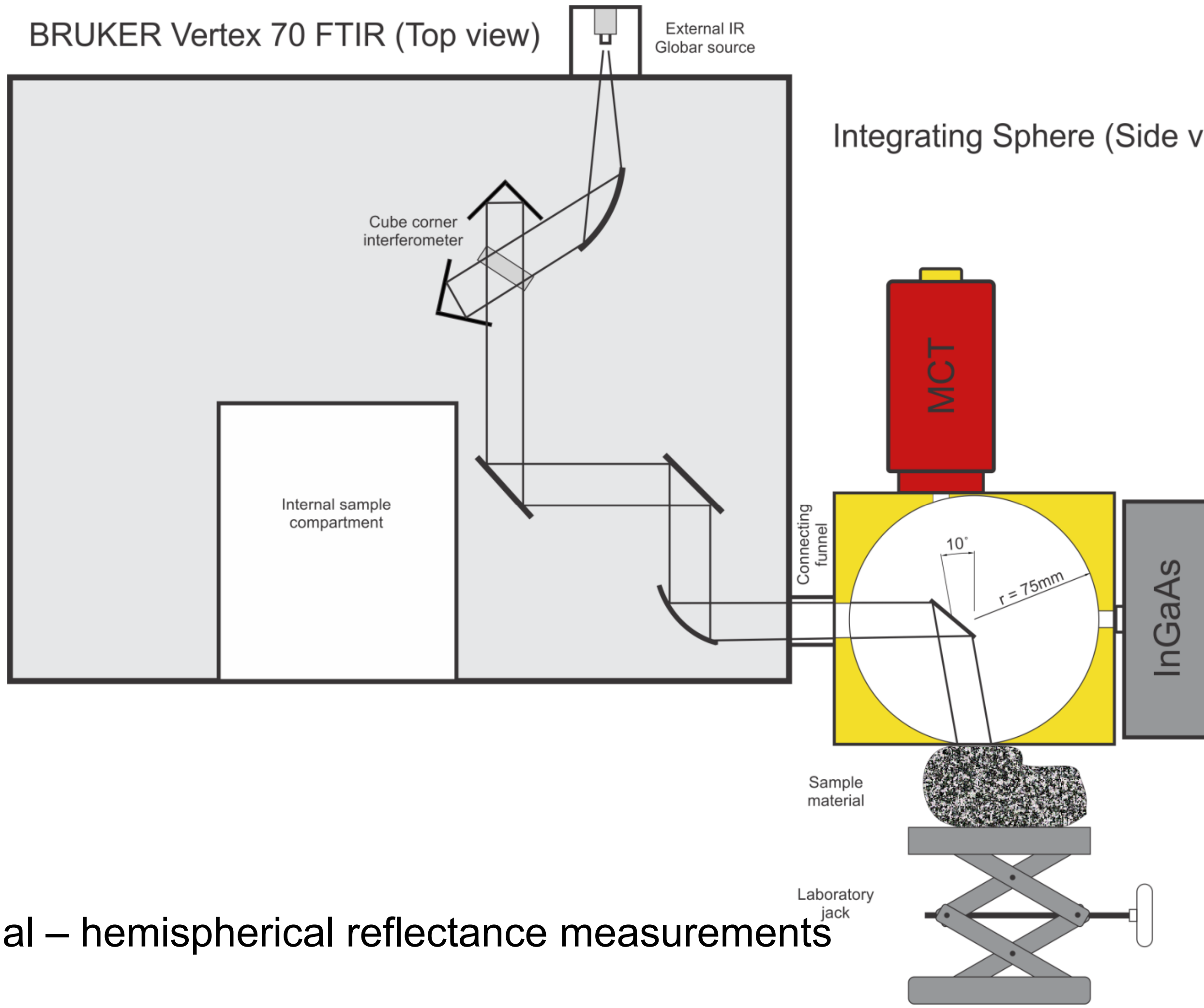
Source: Hecker et al (2010)

EXTERNAL INTEGRATING SPHERE MEASUREMENT

- Gold integrating sphere
- Double source (SWIR & TIR)
- Double detector (SWIR & TIR)
- Large samples from bottom



EXTERNAL INTEGRATING SPHERE MEASUREMENT (CONT'D)



Directional – hemispherical reflectance measurements

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Source: Hecker et al (2011)

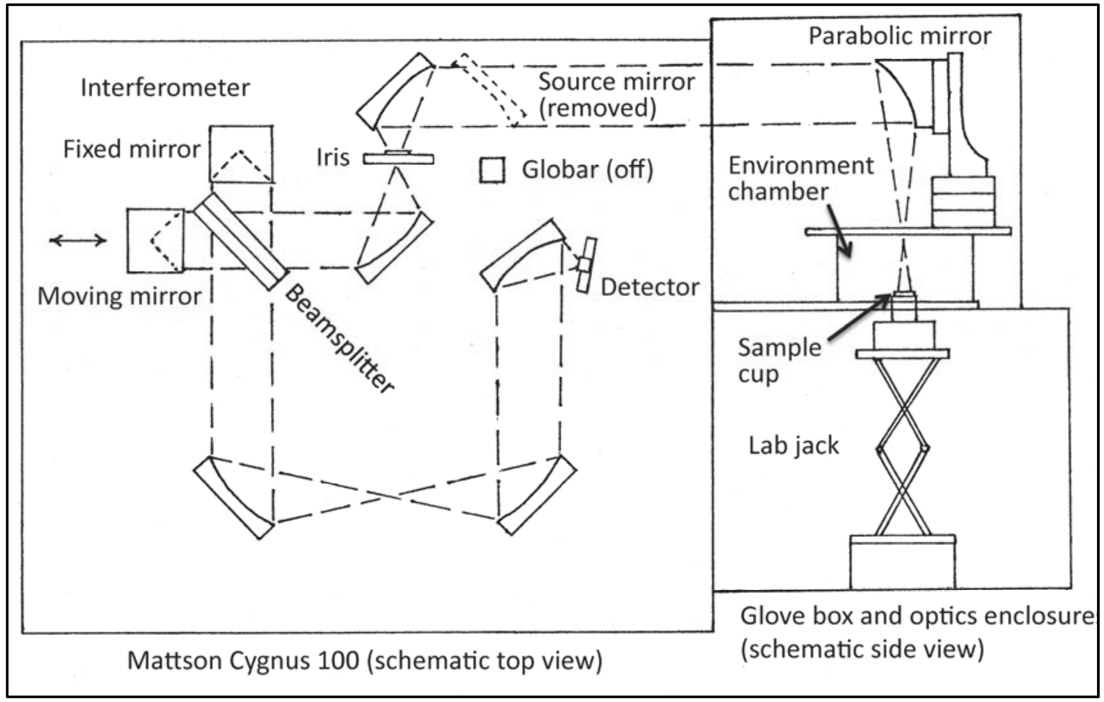
EXTERNAL INTEGRATING SPHERE MEASUREMENT (CONT'D)

Similar setups at JPL (top left), Geologic Survey Japan (top right) and USGS Reston (bottom center).

Photo credit GSJ: R. Hewson

LABORATORY EMISSIVITY MEASUREMENTS

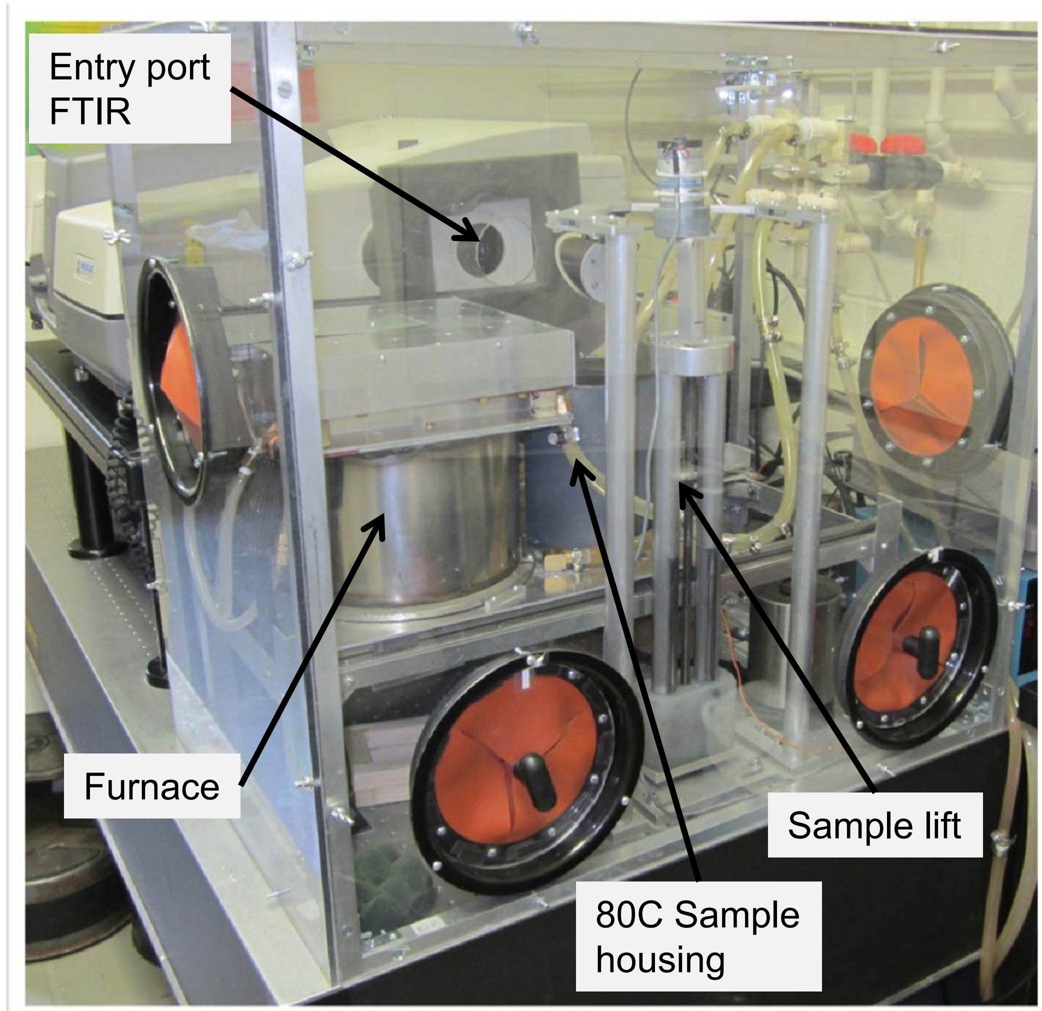
- Schematics of emissive system at Arizona State University
- Planetary community more into emission lab measurements (avoid uncertainty of Kirchhoff law)



(Schematics: Ruff, 1997)

PITTSBURGH EMISSIVE LAB SPECTROMETER

- Prof. Mike Ramsey (formerly ASU)
- Emission system based on ASU but further developed
- Low temp (80C) and high furnace for high temp (up to 1200C)
- Measurement of emissivity changes when rocks melt



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FIELD – INSTRUMENT CONSIDERATIONS

- Weight
- Power consumption
- Temperature stability
- Ruggedness
- Quality of spectra measured
- …
- Applicability to Earth Science samples (most systems for open path / gases).

FIELD – STARTING POINT 1 - μ-FTIR

- Pro:
  - Quite light (ca. 7 kg)
  - Low power consumption
  - Designed with ES in mind (down-looking)
  - Ready-to-go system
- Con:
  - Resolution limited
  - Speed of measurement suite
  - Portability OK but not ideal
  - Not rugged
  - Not certified for Europe

Photo source: Richard Bedell, Auex.com

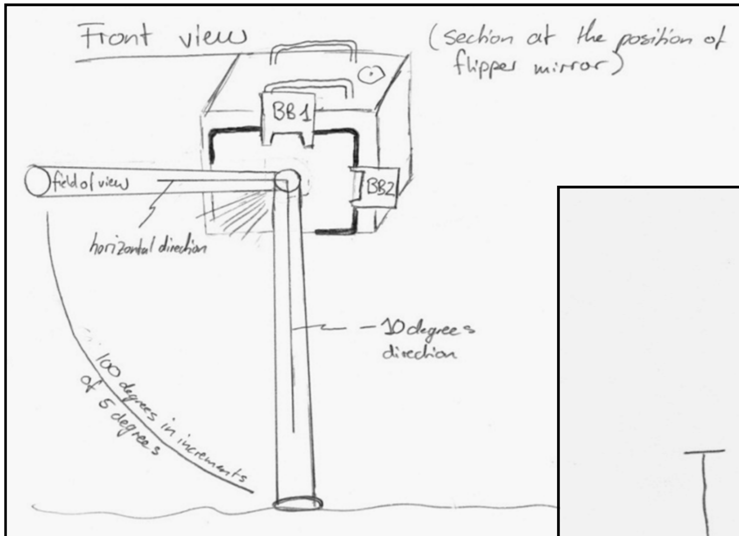
FIELD – STARTING POINT 2 – EMISSION FTIR

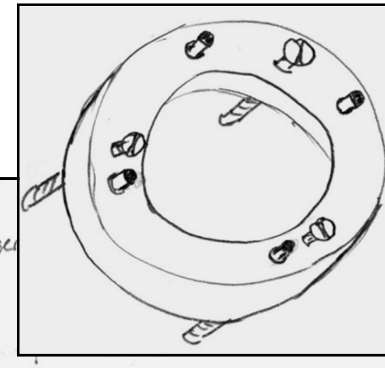
- Pro:
  - High resolution
  - Good quality of spectra (high throughput)
  - Rugged

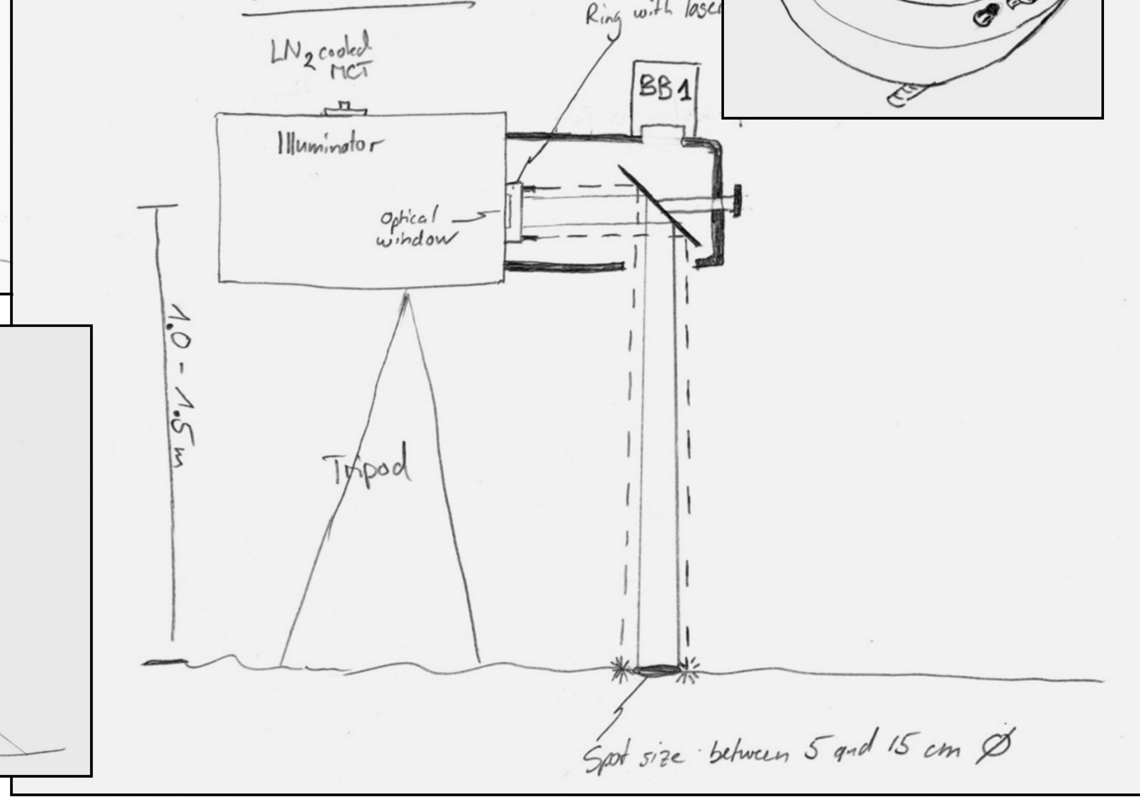
- Con:
  - High power consumption
  - Weight!
  - Made for open path emission measurements. Need specific foreoptics

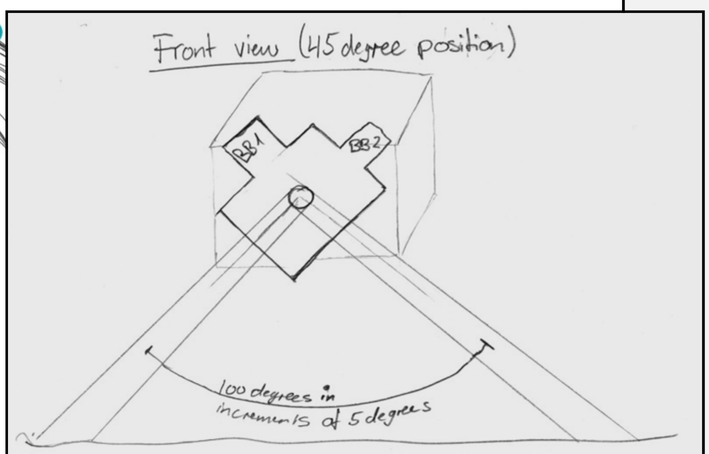
Photo source: C. Oppenheimer

FIELD – CURRENT ITC SOLUTION









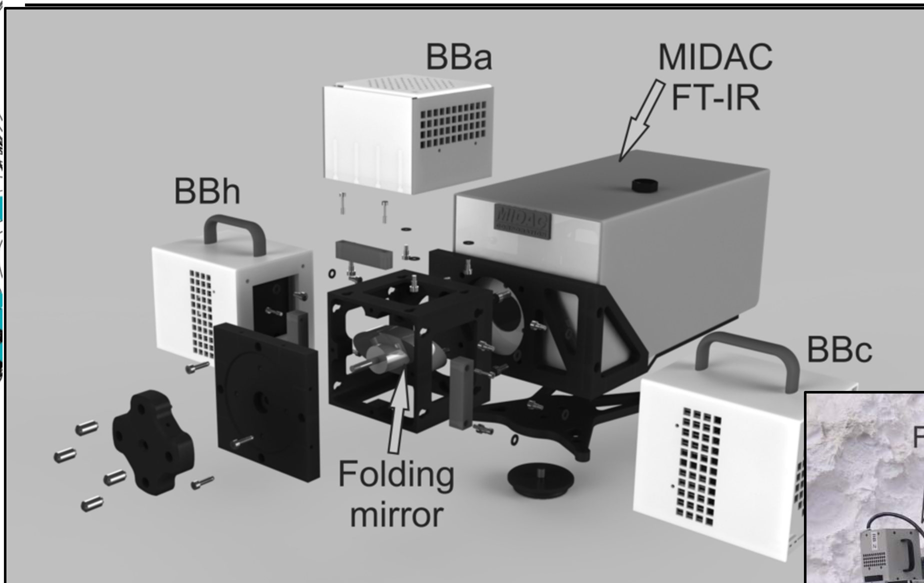
UNIVERSITY OF TWENTE. Lesson: make sure you know what you want

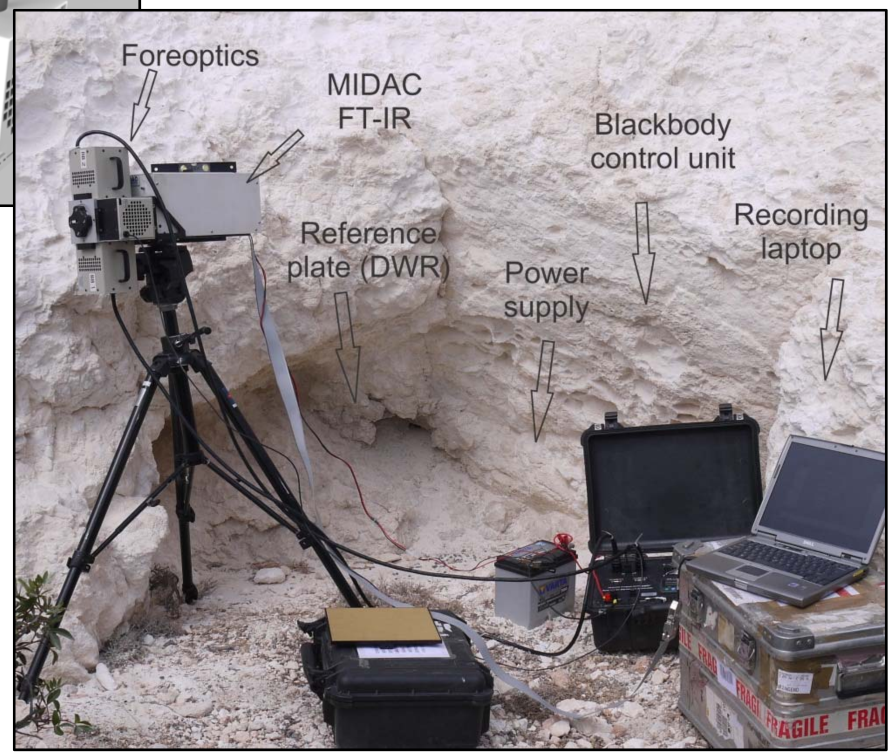
FIELD – CURRENT ITC SOLUTION (CONT'D)

WITH CUSTOMIZED FOREOPTICS

- MIDAC Illuminator M4401
- Non-hygroscopic ZnSe optics
- Heavy duty, sealed cast aluminium housing (ca 15kg)
- lN2 cooled

FOREOPTICS – MARK2





- Next development stage of foreoptics by NERC-FSF.

Photot credit: Chris MacLellan, University of Edinburgh

FIELD IMAGING SPECTROMETER – TELOPS HYPERCAM

- Emissive system
- Imaging FTIR
- Spectral range: 7.7 - 11.5 µm
- Image pixels: 320 x 256
- Calibration: 2 Blackbodies
- Weight: ~30 Kg

AGILENT EXOSCAN 4100

- Diffuse reflectance measurements
- Not quantitatively comparable to emissive systems
- Lightweight: ~3 Kg
- Comparable in use to PXRF

CONSIDERATIONS - LABORATORY

- Decide: speed or absolute emissivity values?
  - Speed: bi-directional (cheap, fast, high SNR)
  - Abs. Emiss: more effort, costs, measurement time

- Abs. Emissivity:
  - Sphere: long measurements, costs (1kEUR per cm diameter)
  - Emission: sample temperature control!

CONSIDERATIONS - FIELD

- TIR field instruments not in ASD-like category
- Decide: 50 kg equipment to field or 50 kg samples to lab?
- Personal take on this question: Bring samples to lab except:
  - Calibration Airborne campaigns
  - Vegetation (?Lichen)
  - Extremely large samples (e.g. entire quarry wall)
  - Undisturbed soils and evaporite crusts (sometimes sample rings possible?)

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MAPPING METHODS

- TIR preprocessing fundamentally different (e.g. TεS)
- After reduction to ground leaving radiance, same hyperspectral tools as VNIR-SWIR mineral mapping, e.g.:
  - Linear unmixing
  - Partial Least Squares Regression (PLSR)
  - Mixture Tuned Match Filter (MTMF)
  - Spectral Angle Mapper (SAM)
  - Feature fitting
  - …
  - etc.

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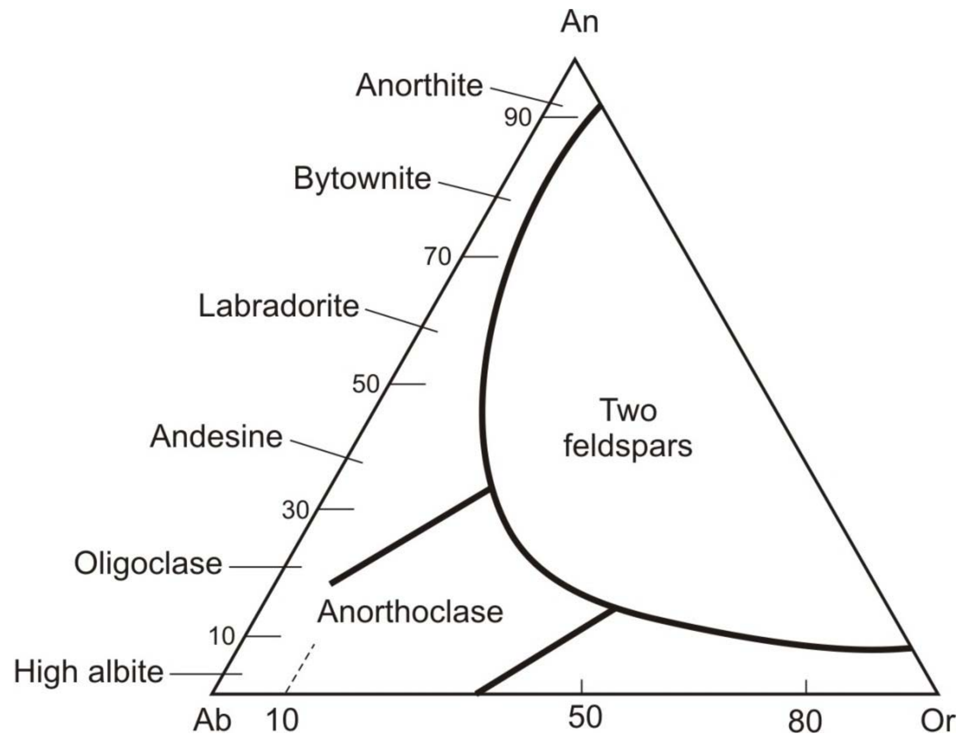
CASE STUDY: TIR – PLSR – MINERAL MODES

- Determining quantitative rock compositions (= “mineral modes”) on lab and airborne TIR spectra.

- Quartz modes

- Alkali feldspar and plagioclase modes

- Plagioclase compositions



Source: Hecker et al (2010)

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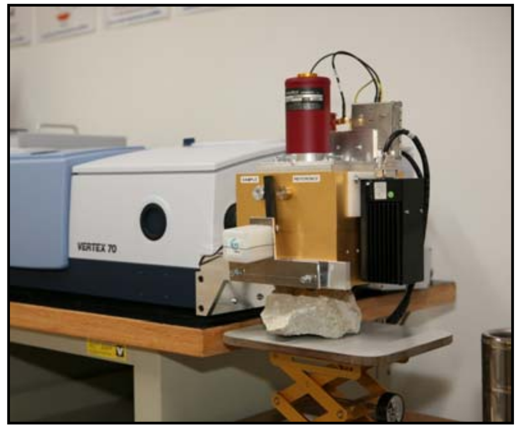
QUANTITATIVE TIR SPECTROSCOPY

LINKING SPECTRA TO MINERALOGY AND MINERAL CHEMISTRY

Thin section blocks

+



Bruker FTIR

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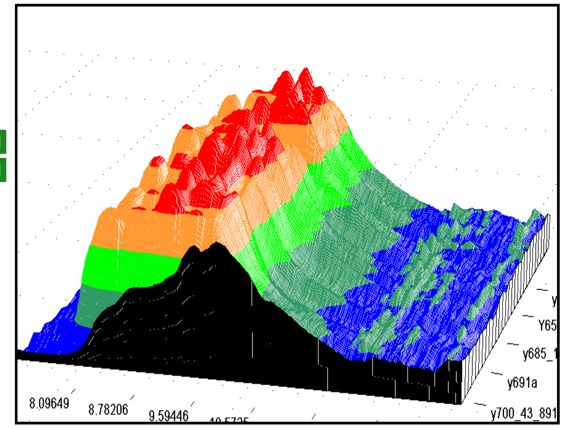
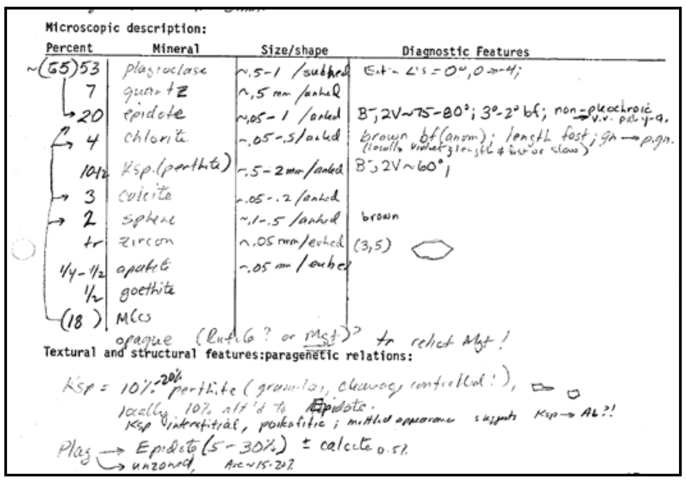


TIR spectra



Microscopic description:

Percent	Mineral	Size/shape	Diagnostic Features
~(55)53	plagioclase	~.5-1 / subhed	Ext. ∠'s = 0°, 0→-4;
7	quartz	~.5 mm / anhed	
20	epidote	~.05-1 / anhed	B⁻; 2V~75-80°; 3°-2° bf; non-pleochroic → v.v. pale y-g.
4	chlorite	~.05-.5 / anhed	brown bf (anom); length fast; gn → p.gn. (locally violet; length fast or slow)
10½	Ksp. (perthite)	~.5-2 mm / anhed	B⁻; 2V~60°;
3	calcite	~.05-.2 / anhed	
2	sphene	~.1-.5 / anhed	brown
tr	zircon	~.05 mm / euhed	(3,5)
¼-½	apatite	~.05 mm / euhed	
½	goethite		
(18)	Mics		

opaque (Rutile? or Mgt)? tr relict Mgt!

Textural and structural features: paragenetic relations:

Ksp = 10%-20% perthite (granular, cleavage controlled!), locally 10% alt'd to Epidote. Ksp interstitial, poikilitic; mottled appearance suggests Ksp → Ab?!

Plag → Epidote (5-30%) ± calcite 0.5%
↳ unzoned, An~15-20%

Thin section description

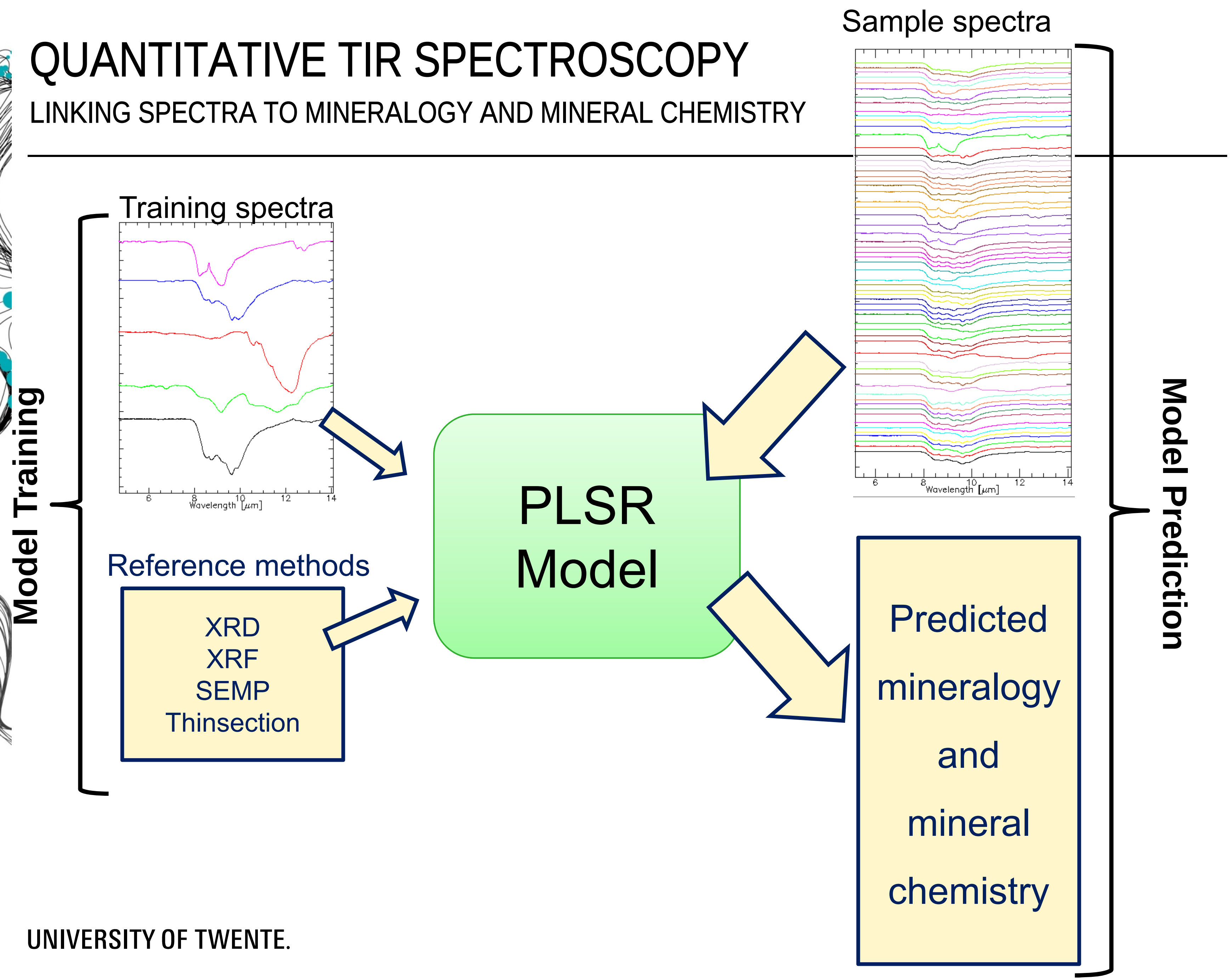
=

sampleloc	lithunit_shpfile	TS_name_long	samplenr	lithunit_Tssheet	alteration	quartz	plagioclase	kfsp	diopside	clinozoisite	garnet	plagcomp	Bt_ign	Bt_2nd	Bt_total
563	Jmd	Y653_90067_26	Y-563	QMD	pervasive S-2 or ES-2	17	70	0	8	1tr		35	0	0	0
653	Jqmp	Y653	Y-653	QMP	wk ab-chl	3	19	4	0	0	0?		0.5	2	2.5
651	Jmd2	y651_16_891	Y-651	Jqmd	?	5	50	16	0	0	strongly 0zoned		0	0	10
48	Jqmp	y48_90067_5	Y-48	GP dike	oli chl rt ep (py)	24	25	24	0	0	0	24	0	0	0
787	Jbqm	y787_11_728	Y-787	?Jpqmj	wk clay	30	35	27	0	0	0	25	0	0	5
692b	Jqmp	y692b	Y-692B	?	wk sericitic	32	27	36	0	0	0	8	0.5	0	0.5
681	Jqmp	y681_40_237	Y-681	Jqmp	wk potassic	5	21	7	0	0	0?		0	1	1
684	Jqmp	y684_41_237	Y-684	Jqmp	wk potassic/ ep+chl	0.5	8	0	0	0	0?	tr		1	1.25
685	Jbqmt	y685_18_891	Y-685	Qz monzodiorite	?	20	35	28	0	0	0	22	0	0	5
688	Jqmp	y688_19_891	Y-688	QMP	?	3	30	3	0	0	0	33	0	0	0
690b	Jbqmt	y690b_42_237	Y-690-B	Jbqmt	wk chl-py-ser / superg clay	30	27	27	0	0	0?		0.25tr		0.25
693a	Jbqm	y693a	Y-693A	Jbqm	? Possibly chl-ser	22	32	31	0	0	0	35	0.5tr		0.5
700	Jbqmt	y700_43_891	Y-700	transitional phase of border qz monozonite	wk Kfsp-clay-ep	35	20	33	0	0	0	29	1	0	1
708b	Jmd	y708b_50_237	Y-708B	Jqmd	wk potassic	10	50	15	0	0	0?		0	10	10
750	Jpqm	y750_LDU-3_thk	Y-750	PG Luhr Hill	fresh	25	35	25	0	0	0	17	6	1	7
665	Jmd	y665	Y-665	QMD	wk SW	10	40	8	0	0	0	20	3	0	3
689	Jmd	y689	Y-689	QMD	Na-Ca	12	45	9	0	0	0	28	3	0	3
690a	Jbqmt	y690	Y-690A	QMD	wk Na-Ca	7	42	12	0	0	0?		0	0	0
691a	Jbqm	y691a	Y-691A	BG	PA	30	22	32	0	0	0	24	6	0	6
691b	Jbqm	y691b	Y-691B	QMD	wk PA	6	55	6	0	0	0	7	0	0	0
46	Jqmp	y46_90067_4	Y-46	GP dike	Phlogo-Chl-Ep	0.25	25	0	0	0	0	26	0	0	0
320	Jmd	y320_90067_11	Y-320	QMD	Act / Ep	9	50	9	0	0	0	0tr		0tr	
321	Jmd	y321_90067_12	Y-321	QMD	wk ES	10	55	12	5	0	0	25	3	0	3
323	Jbqm	y323a_90067_12	Y-323A	BG	wk PA	29	26	29	0	0	0	24	8	0	8
323	Jbqm	y323b_90067_14	Y-323B	Andesite Dike	?	1	65	0	0	0	0?		0	0tr	
335	blueHill	y335_grinding_b	Y-335	?Andesite; Arthesia	?	0	65	0	0	0	0	10	0	0	0
680b	Jqmp	y680b_13_237	Y-680-B	Jqmp	?	1	24	0	0	0	0	29	0	0.25	0.25
692d	Jdqmt	y692d_43_237	Y-692D	Jbqm(t)	Qz-Tm-Ser	32	21	27	0	0	0	32	0.125	4.5	4.625
797	Jmd	y797_15_7	Y-797	Artesia Fm	wk Ep-clay-Ab	0	53	0	0	0	strongly zoned and several generation 0s		0	0	0

TS descr. In Spreadsheet

QUANTITATIVE TIR SPECTROSCOPY

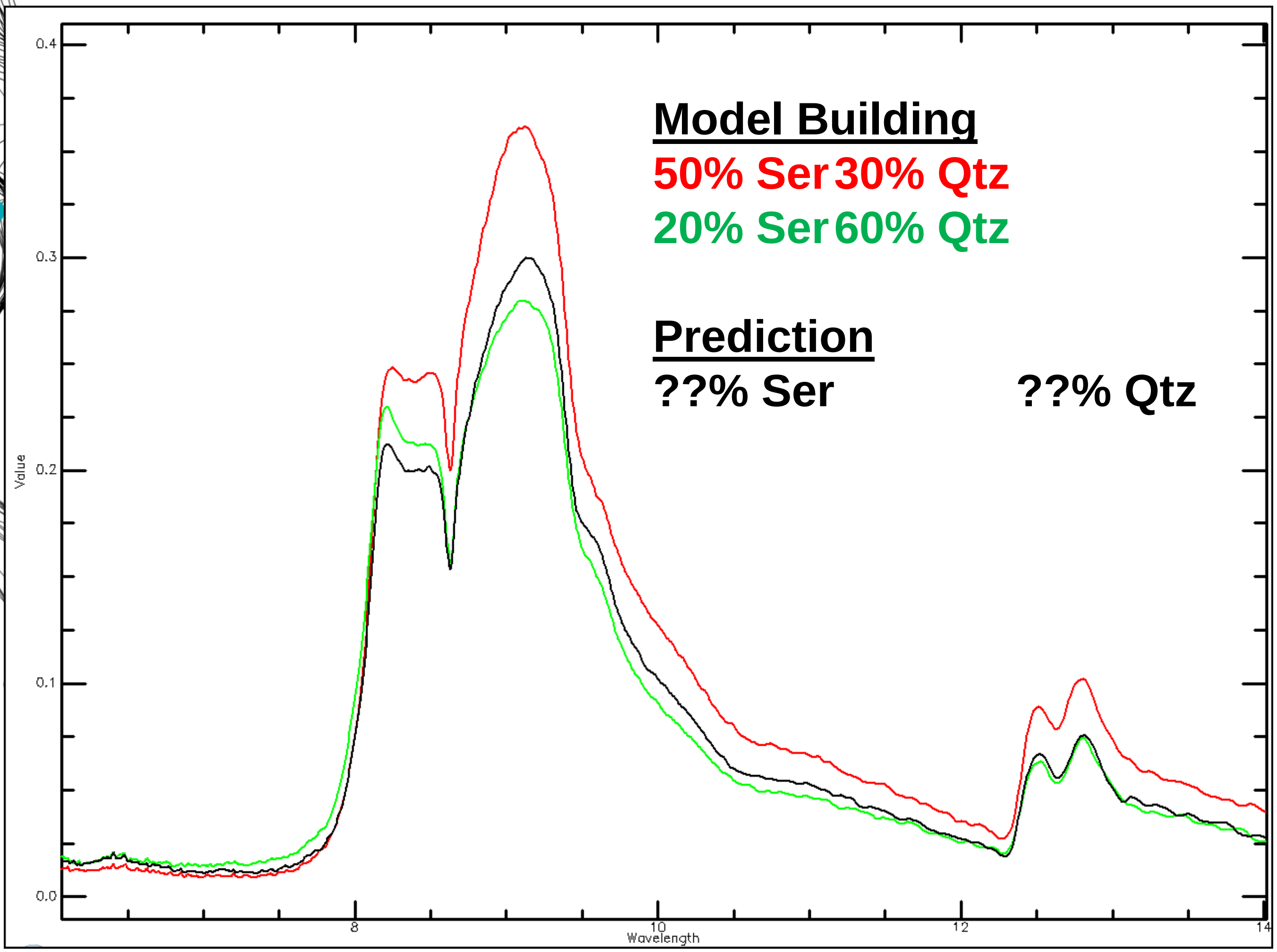
LINKING SPECTRA TO MINERALOGY AND MINERAL CHEMISTRY



WHAT IS PLS?

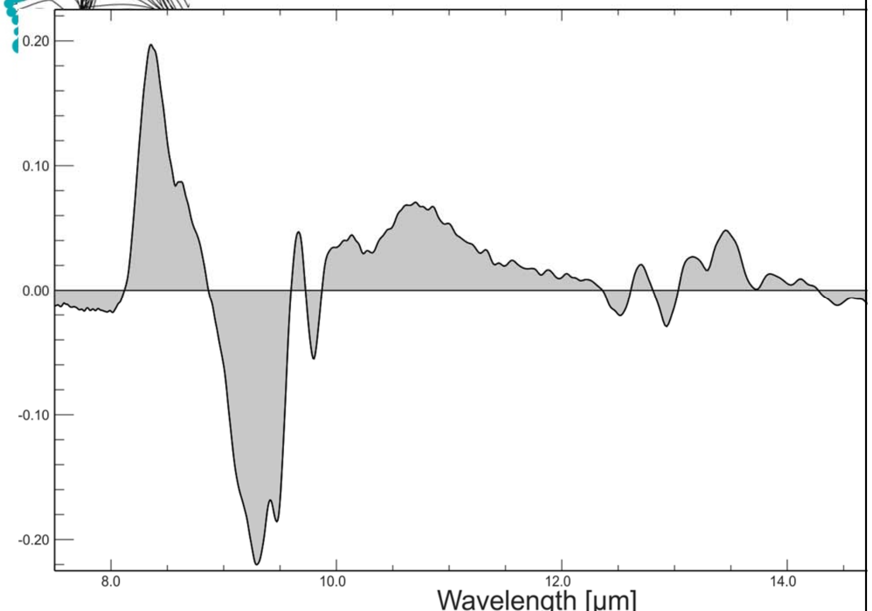
- Regression method
- Links attribute data to spectra
- Decomposes into components similar to Principal Component Analysis
- Good for spectroscopy:
  - Compresses info into a few components
  - Can deal with lots of bands and selects the most important
  - Deals well with correlated attributes (adjacent bands often 99% correlated)

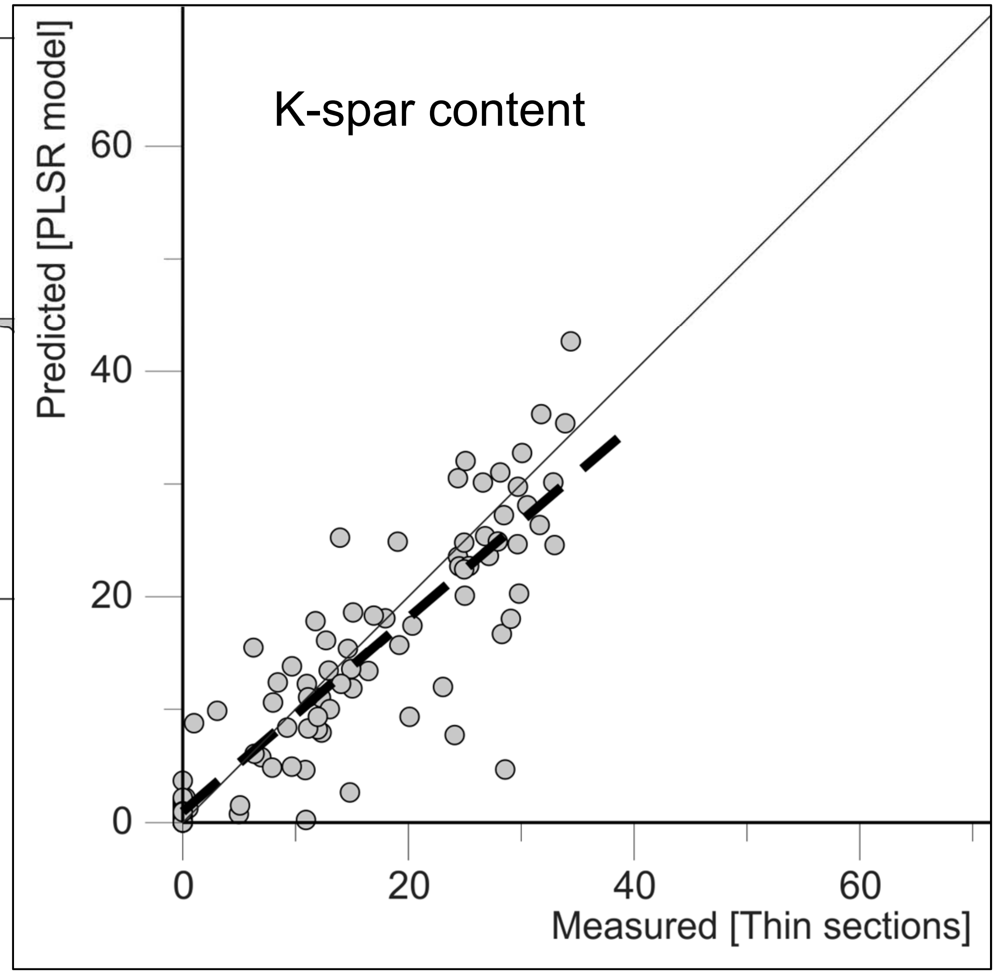
SIMPLIFIED PLS EXAMPLE



PLSR ON TIR SPECTROSCOPY

PREDICTION RESULTS



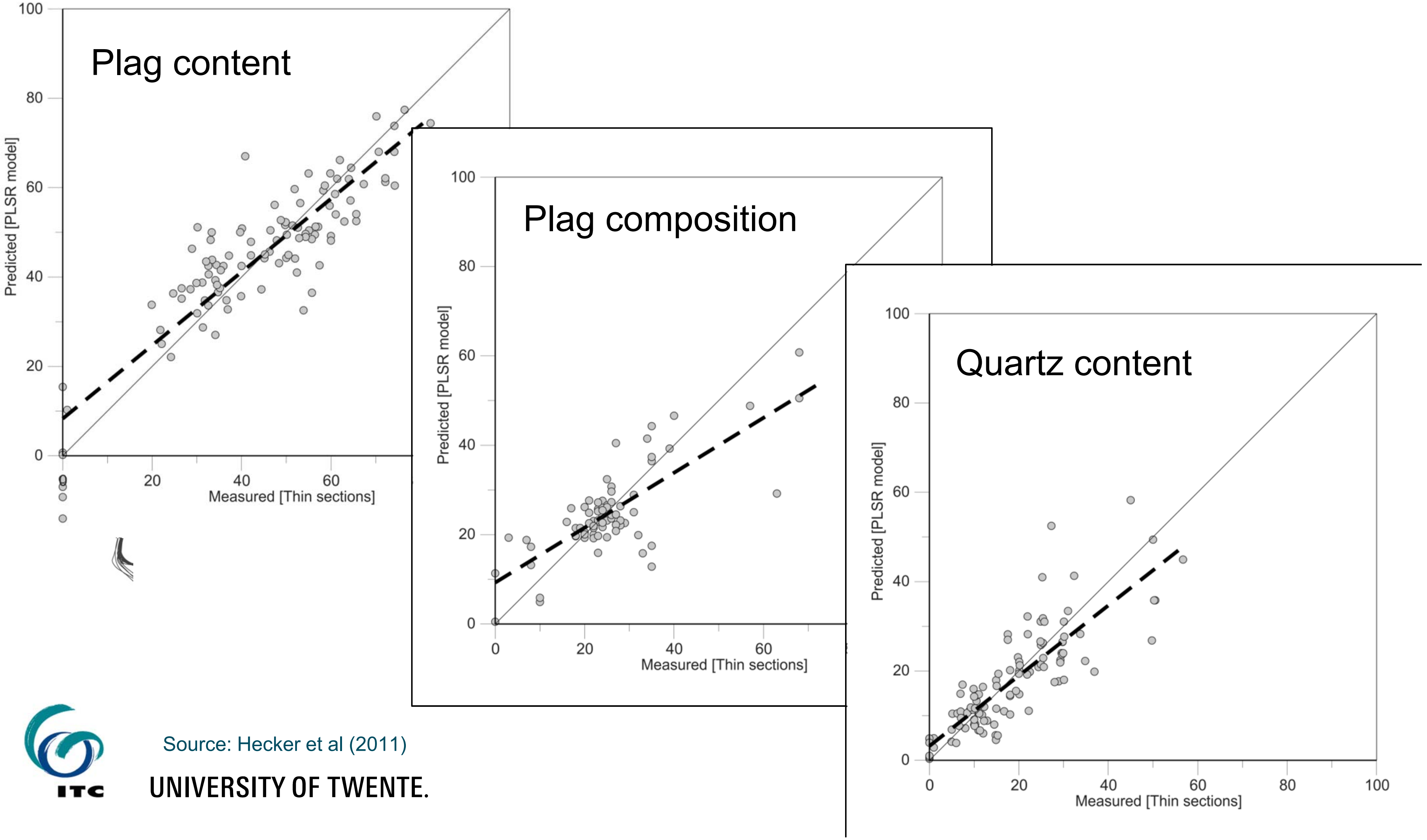


- Regression coefficients and meas. vs. predicted plot

Source: Hecker et al (2011)

PLSR ON TIR SPECTROSCOPY

PREDICTION RESULTS



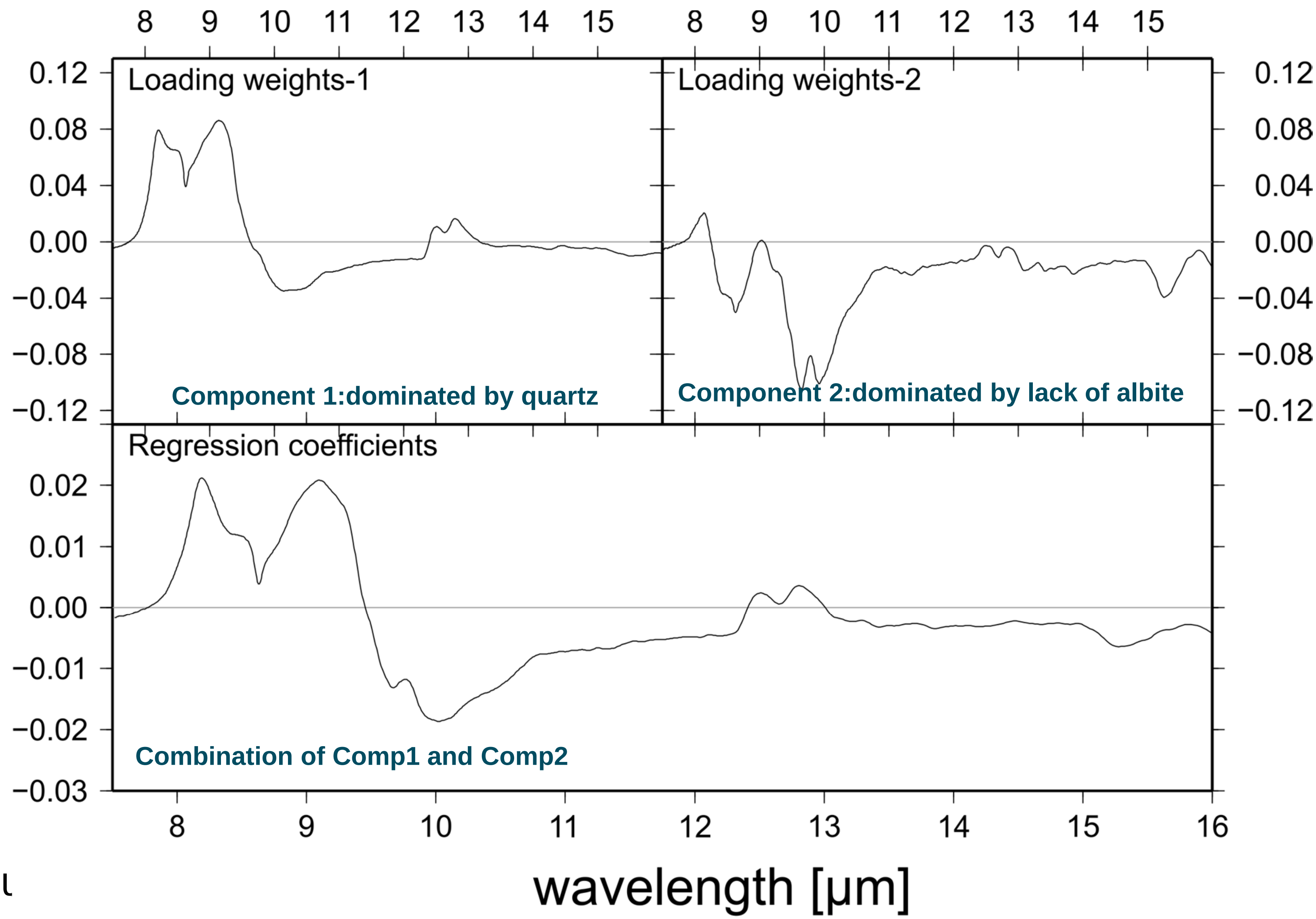
Source: Hecker et al (2011)

PLSR ON TIR SPECTROSCOPY
PREDICTION RESULTS

Mineral	Ksp	Plg	Qtz	Plgcomp
Number of LV's used	5	4	2	5
RMSEP [in %abs]	5.13	8.52	6.90	7.79
R2	0.81	0.80	0.70	0.59
slope (of regression line)	0.86	0.82	0.79	0.61

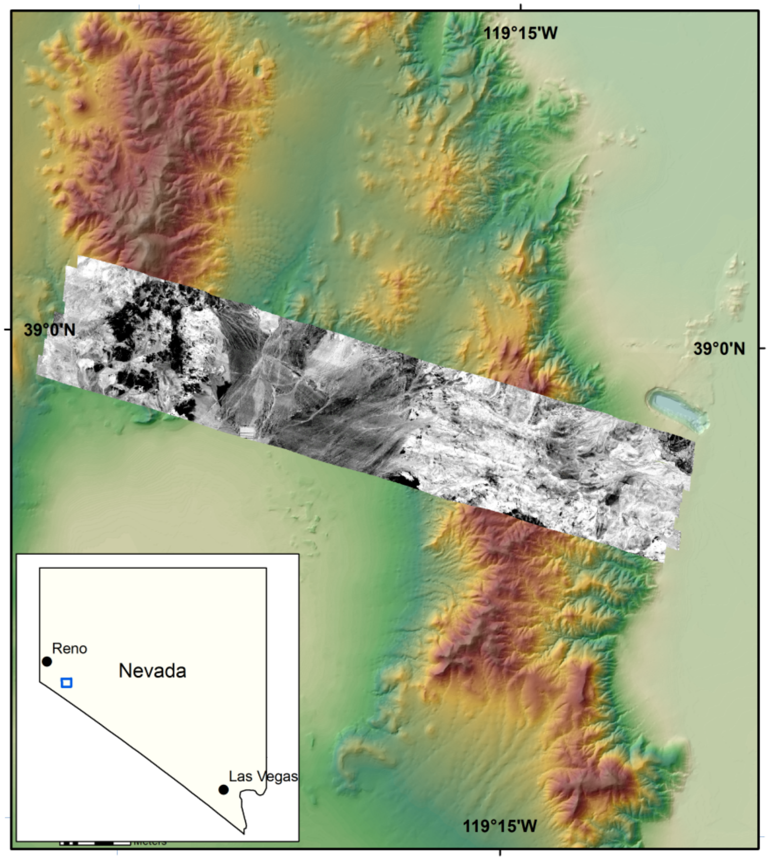
PLSR ON TIR SPECTROSCOPY

MODEL INTERPRETATION (CASE OF QUARTZ)



APPLICATION TO AIRBORNE HYPERSPECTRAL IMAGE DATA

AEROSPACE CORPORATION'S SEBASS SENSOR OVER YERINGTON BATHOLITH, NEVADA



Data courtesy Dr. Dean Riley, Aero.org

THE AEROSPACE CORPORATION

ITC

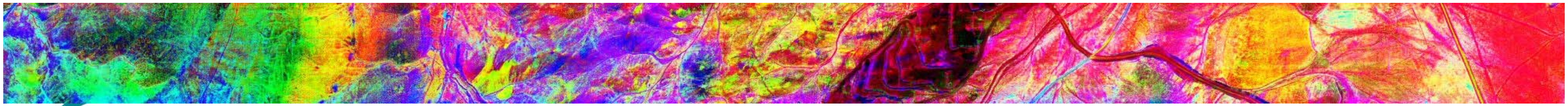
UNIVERSITY OF TWENTE.

Source: http://www.lpi.usra.edu/science/kirkland/Mesa/text.html

YERINGTON FIELD IMPRESSIONS

Yerington Mine (porphyry Cu)

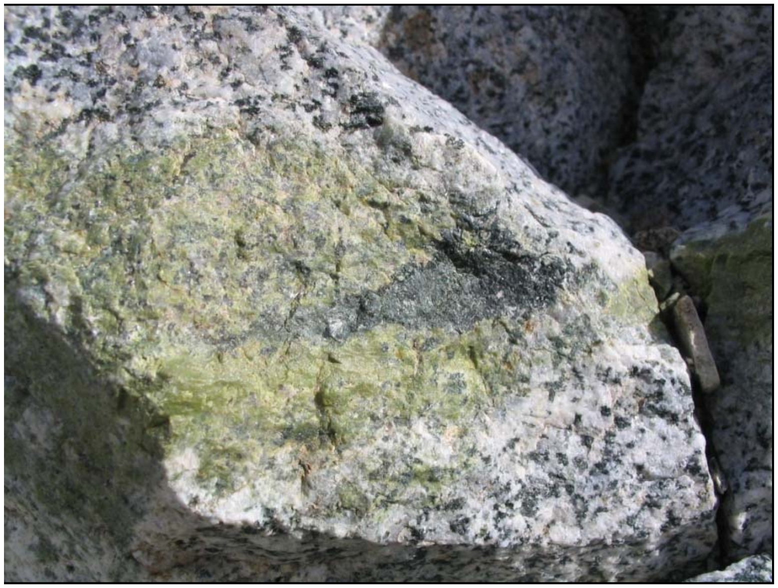
MacArthur Mine (porphyry Cu)



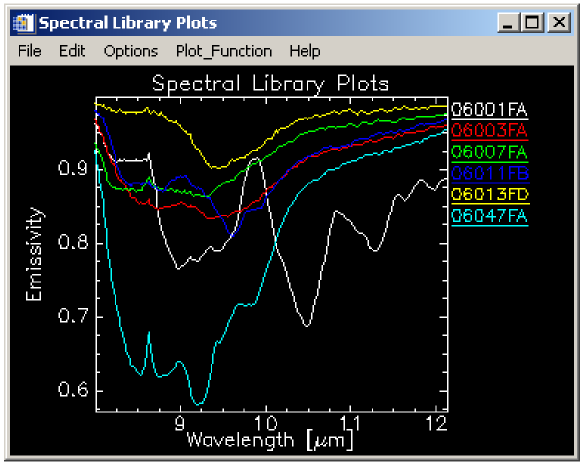
SEBASS d-stretched Colour Composite

YERINGTON FIELD IMPRESSIONS (CONT'D)

Breccia with Cu-Oxides

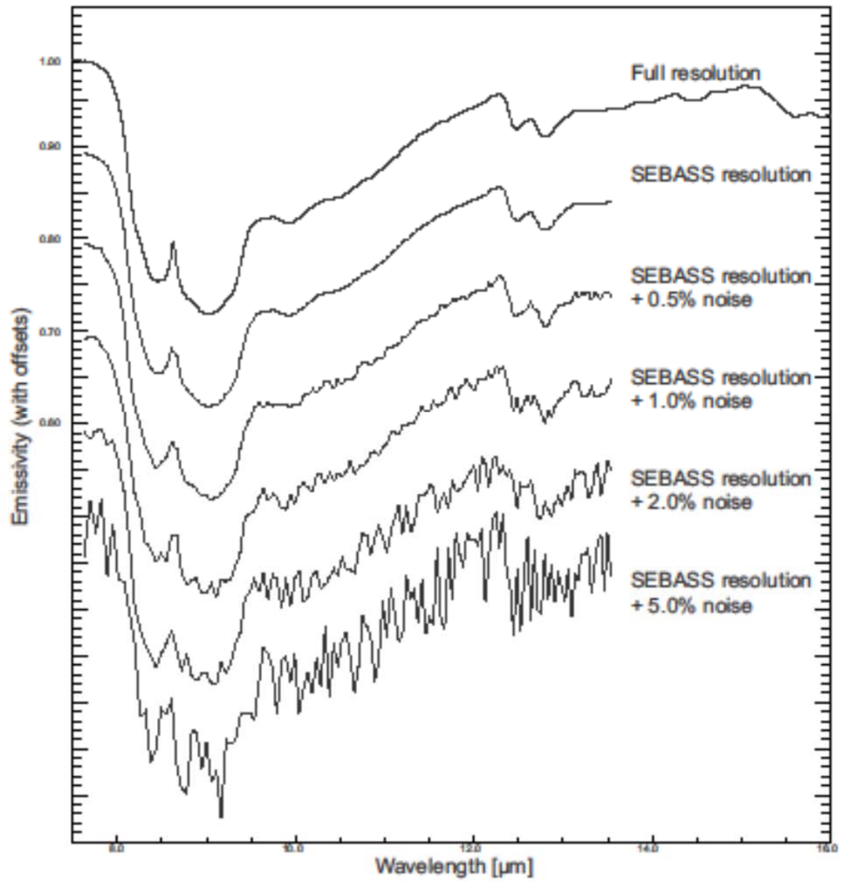


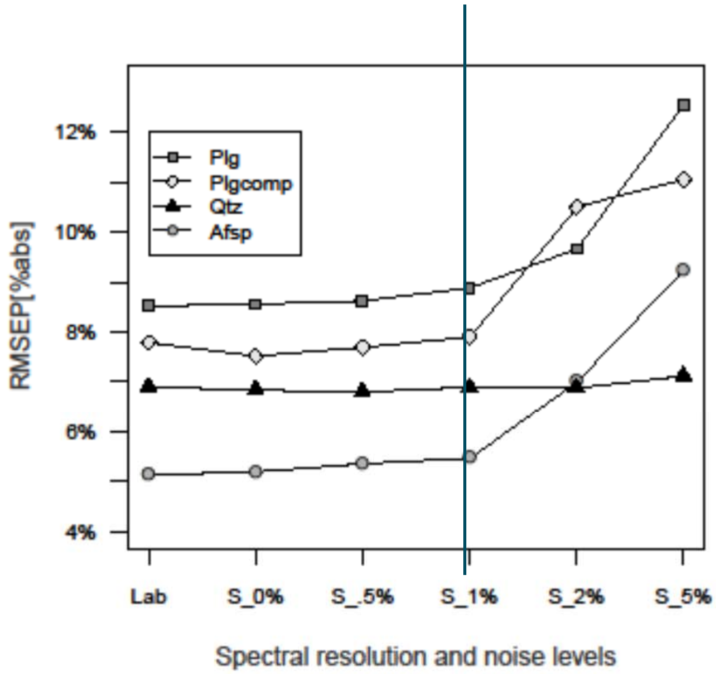
Granite w/ Epidote and Hornblende



MODELING FIRST

- Adding noise up to 1% (absolute) to emissivity spectra gives OK results

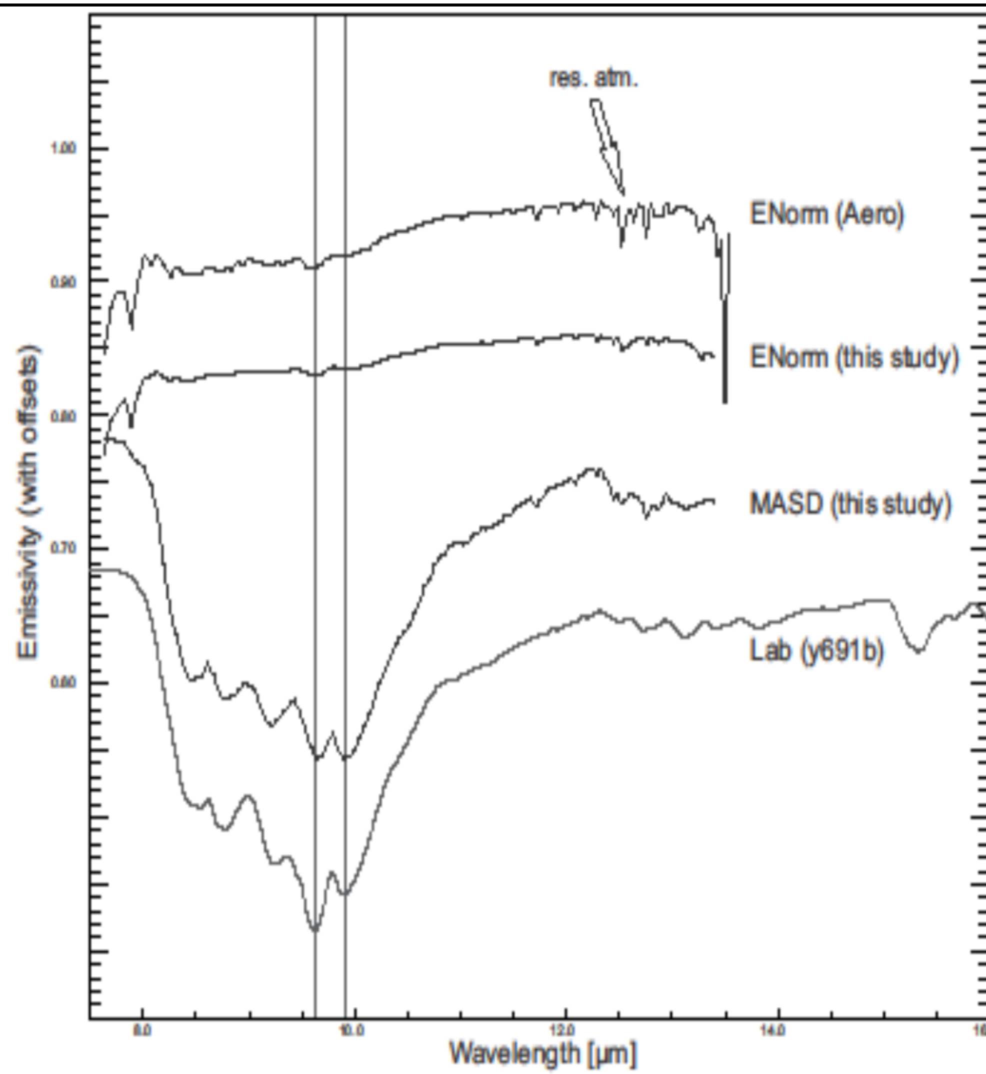




Source: Hecker (2012)

NORMALIZING SPECTRAL CONTRAST

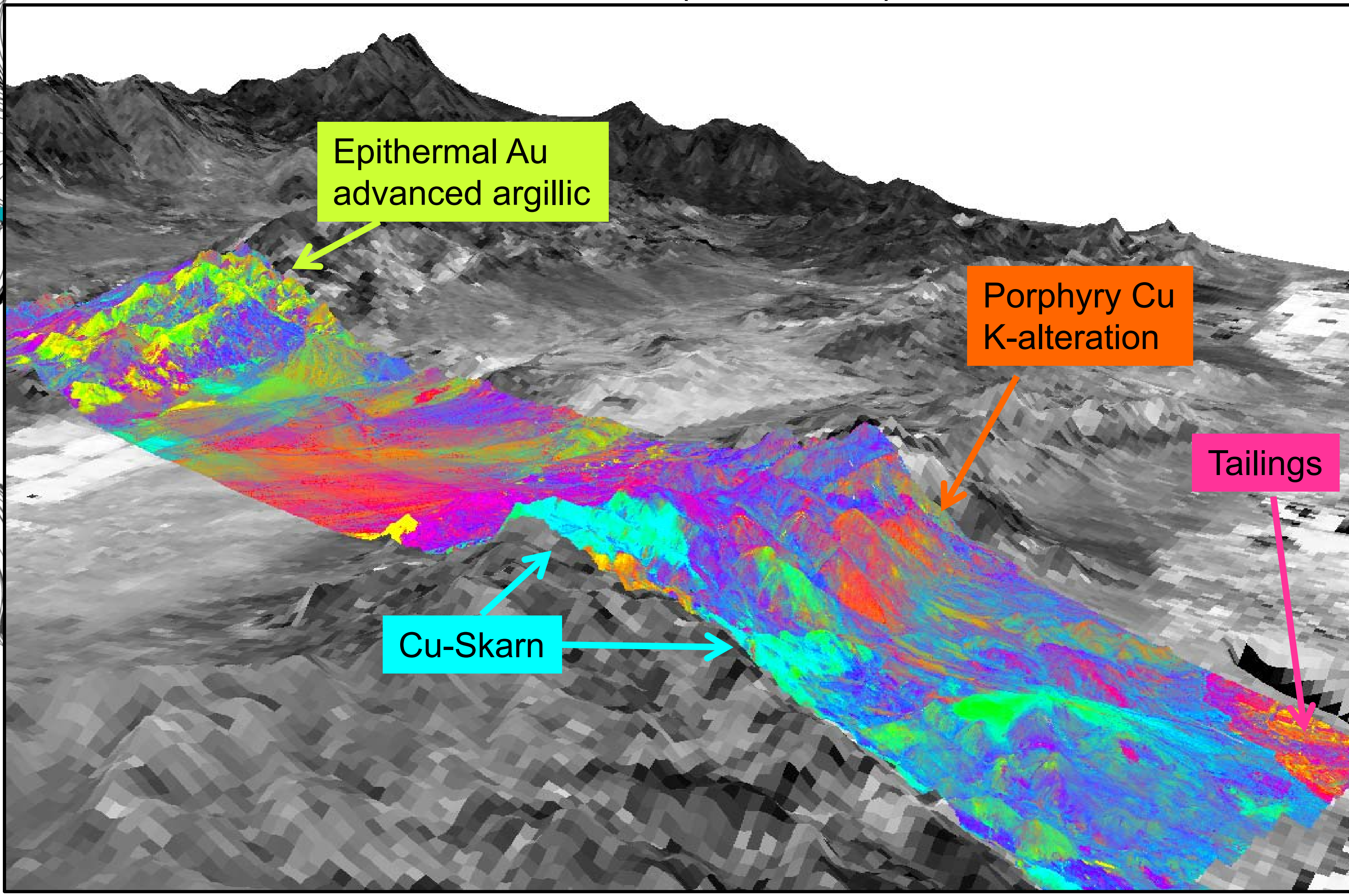
- Airborne spectra have minimal spectral contrast
- For quantitative results, spectral contrast needed normalization.



Source: Hecker (2012)

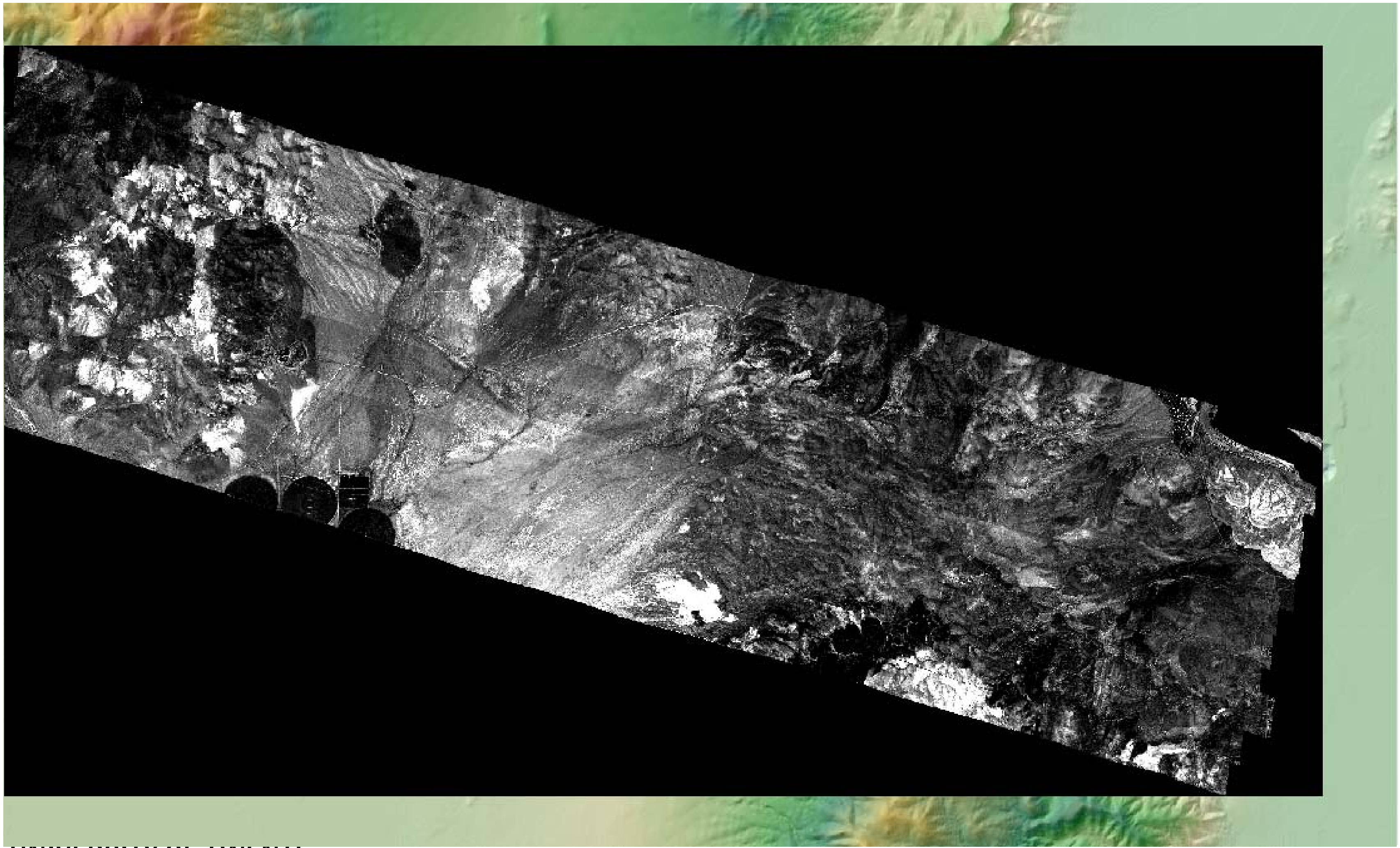
AIRBORNE HYPERSPECTRAL IMAGING

YERINGTON TIR COLOUR COMPOSITE RGB = (11.1, 9.64, 9.06)



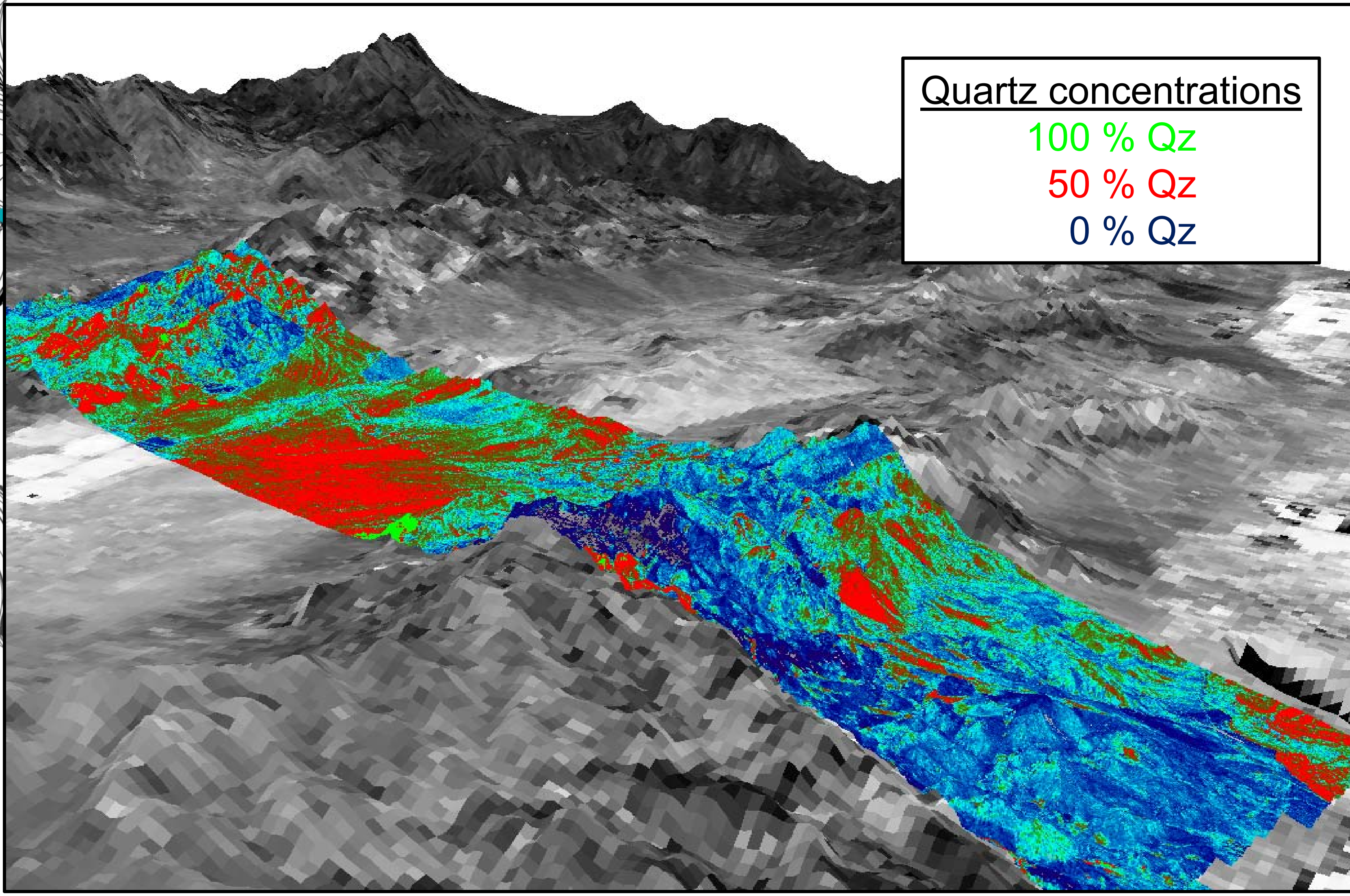
QUANTITATIVE AIRBORNE ANALYSIS

APPLYING PLS MODEL TO AIRBORNE DATA – QTZ CONCENTRATION AS GRAYSCALE IMAGE



QUANTITATIVE AIRBORNE ANALYSIS

APPLYING PLS MODEL TO AIRBORNE DATA – DENSITY SLICED



SOURCES OF ADDITIONAL INFORMATION:

TEXTBOOKS WITH TIR CHAPTERS

- **C. Kuenzer und S. Dech (Eds.)** Thermal Infrared Remote Sensing: Sensors, Method, Applications (2013)
- **Drury** (2001): Image Interpretation in Geology (3rd Edition); Chapter 6
- **Lillesand & Kiefer** (2000): Remote Sensing and Image Interpretation (4th Edition); Chapter 5
- **Sabins** (1997): Remote Sensing – Principles and Interpretation (3rd Edition); Chapter 5
- **Abrams et al** (2001): Imaging Spectrometry in the Thermal Infrared; in vander Meer & de Jong (2001): Imaging Spectrometry; Chapter 10
- **The Remote Sensing Tutorial**
  http://www.fas.org/irp/imint/docs/rst/
  Section 9
- **Gupta** (2003): Remote Sensing Geology (2nd Edition); Chapter 9

SOURCES OF ADDITIONAL INFORMATION:

ARTICLES AND CHAPTERS MENTIONED IN TEXT

- **Hecker et al. (2013)** Thermal Infrared Spectroscopy in the Laboratory and Field in Support of Land Surface Remote Sensing. http://dx.doi.org/10.1007/978-94-007-6639-6_3
- **Riley and Hecker (2013)** Mineral Mapping with Airborne Hyperspectral Thermal Infrared Remote Sensing at Cuprite, Nevada, USA, http://dx.doi.org/10.1007/978-94-007-6639-6_24
- **van der Meer et al. (2012)** Multi - and hyperspectral geologic remote sensing : a review. http://dx.doi.org/10.1016/j.jag.2011.08.002
- **Hecker et al. (2012)** Thermal infrared spectroscopy and partial least squares regression to determine mineral modes of granitoid rocks. http://dx.doi.org/10.1029/2011GC004004
- **Hecker et al. (2011)** Thermal infrared spectrometer for earth science remote sensing applications : instrument modifications and measurement procedures. http://dx.doi.org/10.3390/s111110981
- **Hecker et al. (2010)** Thermal infrared spectroscopy on feldspars : successes, limitations and their implications for remote sensing. http://dx.doi.org/10.1016/j.earscirev.2010.07.005

QUESTIONS??