Spectral Imaging

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Overview

- What is spectral imaging?
- What can we learn from spectral imaging?
- Different types of spectral imaging devices
- Instrument specification considerations
- Calibration & post-processing – an important step in quantitative spectral imaging
- Material identification using spectral reflectance
- The Big Data challenge & modern statistical methods for information extraction – automated uncovering of any 'hidden' features
- Combination with other non-invasive techniques – a systematic approach to non-invasive investigation

Reflectance spectroscopy & spectral imaging

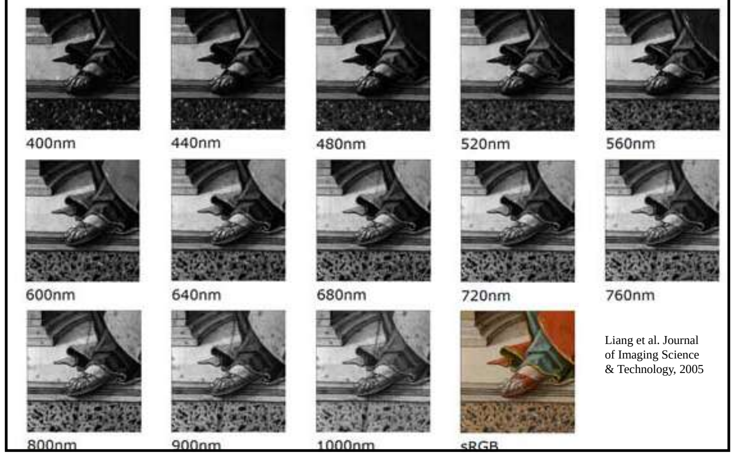
- Spectral imaging is an efficient way of collecting reflectance spectra
- Spectral imaging collects many reflectance spectra simultaneously usually at a lower spectral resolution than reflectance spectroscopy (high spectral resolution)
- Multispectral image – small number of spectral bands (low spectral resolution)
- Hyperspectral imaging – large number of spectral bands (medium spectral resolution)

Fibre optic reflectance spectrometer (FORS) collects one spectrum at a time

- Spectral reflectance is the percentage of light reflected back from a sample
- Spectral imaging can be used for imaging irradiance (emission), transmittance and reflectance

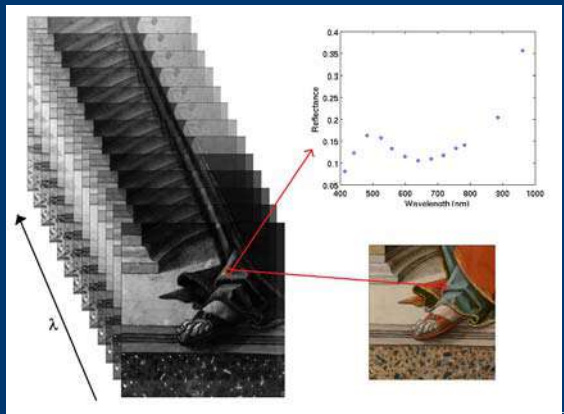
Spectral imaging = multispectral + hyperspectral imaging

Spectral imaging



Liang et al. Journal of Imaging Science & Technology, 2005

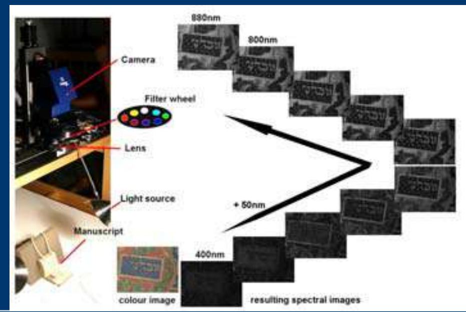
Spectral Imaging Cube



Liang, Applied Physics A, 2012 - a review of spectral imaging

Sequential imaging in spectral bands Simultaneous spatial imaging

- Use filters –captures entire field of view in one go, captures individual bands sequentially



Simultaneous imaging in all spectral bands Sequential spatial imaging

Use gratings – captures entire spectral range in one go for one spatial column, captures the spatial information sequentially column by column

Spectrograph: slit, grating, order sorting filter, relay optics

Filter based versus grating based systems

filter

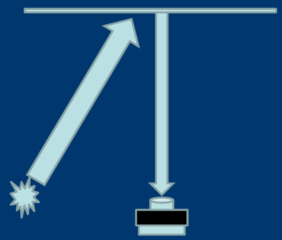
- Low demand on optics – lens only need to be achromatic over the narrow spectral band
- Uniform signal to noise per spectral band
- Natural choice for multispectral imaging where spectral resolution is low
- Not suitable for fast changing samples or environment

grating

- High demand on optics – lens need to be achromatic over the entire spectral range
- Difficult to achieve uniform quality image for all bands
- Natural choice for high spectral resolution, large number of bands
- Can cope with fast changes in the field of view

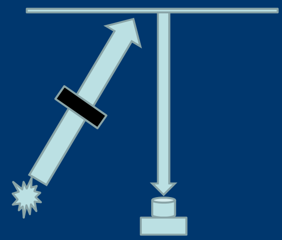
Types of spectral imaging

- Wavelength selection on detector side



Types spectral imaging

- Wavelength selection on illumination side



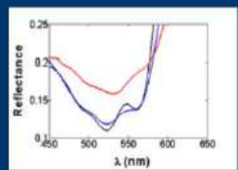
Instrumental design options

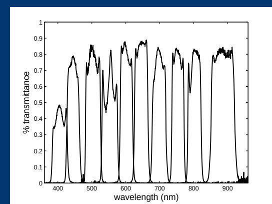
Wavelength selection options:

- –Filter illumination
- –Filter just before detector
  - Filter wheel and interference filters (spectra collected sequentially)
  - Tunable filters: LCTF (Liquid Crystal Tunable Filters), AOTF (Acousto-Optic Tunable Filters), Fabry-Perot elaton (spectra collected sequentially)
  - Slit + Diffraction grating or prisms (spectra collected simultaneously)
  - Michelson interferometers

Spectral resolution requirements

- Optical resolution versus sampling spectral resolution
- Most natural material have smooth spectra – no need for high spectral resolution (10 nm spectral resolution and 5nm sampling interval sufficient for all pigments; 50nm resolution is sufficient for the majority of pigments)
- High spectral resolution means longer exposure time or lower signal to noise for the same exposure time





Scale insect dyes (e.g. cochineal, lac) need the highest spectral resolution/sampling (10nm resolution, 5nm sampling)

Spatial resolution

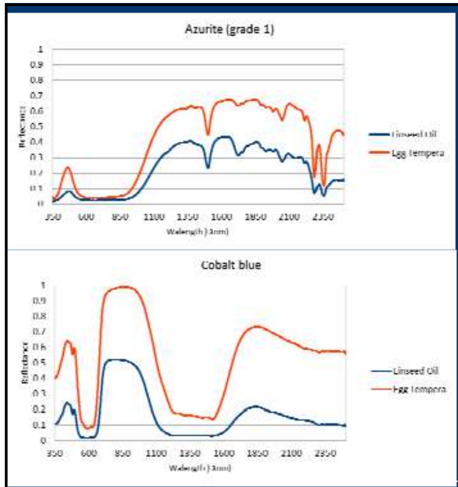
- Optical resolution (real resolution) versus sampling resolution
  - High number of pixels means high sampling resolution but not the actual resolution! You need good optics (lens) to achieve high resolution and high image quality
- Required resolution depends on application, e.g. 25-50 microns gives high enough image quality for imaging of brush strokes

Spectral range

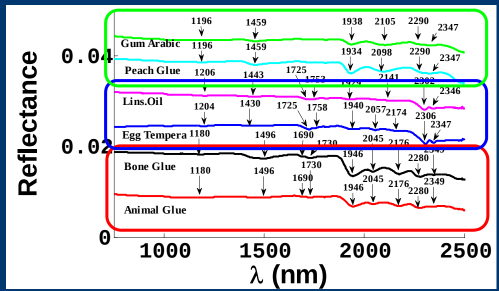
- UV/VIS/NIR: ~350nm to ~1000nm, Si CCD based detector
- SWIR: 1000 nm – 2500 nm, InGaAs, MCT or InSb detectors
- MWIR: 3000 nm – 5000 nm, InSb detectors
- LWIR (FTIR range): 7 – 14 microns, MCT detectors

What information can we get through different wavelength range?

- UV/VIS/NIR (~350-1000nm): characteristic spectral feature of the pigments
- SWIR (1000–2500 nm): additional spectral features for some pigments (e.g. azurite, cobalt containing pigments), information on the binding medium, detection of moisture
- MWIR/LWIR (FTIR range): identification of molecular bonds

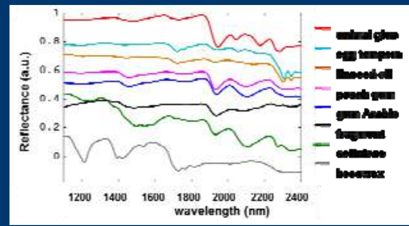


Binding Medium Identification in the SWIR range

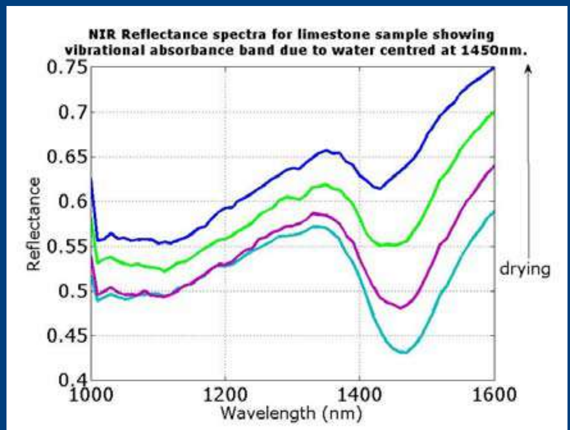


Binding medium identification

Caution: always take into account the effect of substrate and pigments
e.g. difficult to identify animal glue in the SWIR range on paper substrate or in the presence of azurite



Kogou et al., Heritage Science 2016



Standard calibration procedure for quantitative digital imaging

- Dark subtraction: subtract instrumental dark current for each frame
- Flatfield: calibrate the inhomogeneity of the illumination and vignetting of the optical system by imaging a smooth and diffuse white target

Dark current

- Semi-conductor detector at a non-zero temperature will be subject to thermal agitation which can eject valence electrons into the conduction band which is then collected and read out, i.e. electrons are readout in the absence of photon illumination
- These charges can accumulate over time => dark current increases with 'exposure time'
- It is temperature dependent => cooling of CCDs are very important
- CCDs can be cooled by thermal electric methods to -20 to -100 degrees C

Linearity of a CCD

- CCDs are highly linear in intensity compared with older technology such as photographic plates (linear means increasing the intensity by x times will result in the detector registers x times the number of counts)
- Close to saturation CCDs can deviate from linearity (high quality CCDs are made such that saturation level occurs before deviation from linearity)
- Small deviation from linearity can occur close to zero photon exposure

Spectral calibration of filter based systems

- Spectral calibration: image a standard spectral white target through each filter

Note:

For pigment identification, we only need good spectral calibration, but for accurate colour imaging we need the full absolute calibration

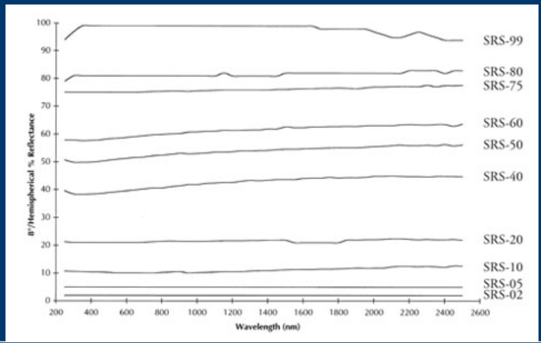
For monitoring spectral change, relative calibration is sufficient, i.e. relative position of target, illumination and detector is fixed.

Calibration standards for imaging reflected light

- Spectral standards
  - white standard with known spectral reflectance over a broad spectral range usually covering the visible/NIR spectral range

- Matt white chart (larger than the field of view) for flatfield calibration to correct for spatial inhomogeneity of illumination, vignetting of optical system (spatial inhomogeneity of optical throughput), pixel-to-pixel gain variation of the CCD

Spectral reflectance of diffuse Spectralon standards



Calculating spectral reflectance

- Calibrated image

<final object frame>

=(<object frame> - <dark frame>)/<normalised dark subtracted flatfield frame>

where <normalised dark subtracted flatfield frame>

=<dark subtracted flatfield frame>/mean(<dark subtracted flatfield frame>)

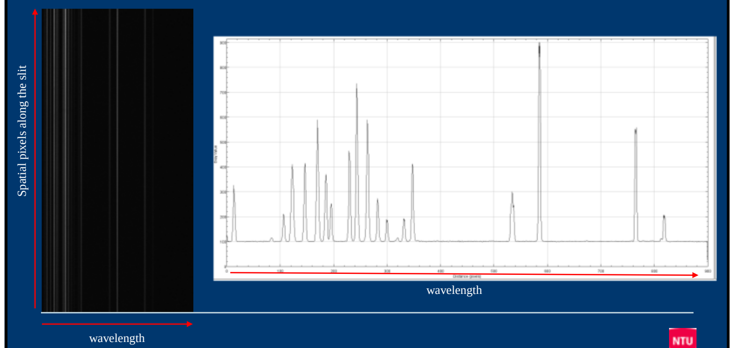
- Reflectance image per channel

= (<final object frame>/t_obj) / (mean(<final spectral white frame>)/t_white)

Where <final spectral white frame> is calibrated in the same way as <final object frame>, t_obj and t_white are the exposure times for the object and spectral white standard frames, the mean should be taken from the central areas of the spectral white image if the field of view is larger than the spectral white standard itself

Spectral calibration for grating based hyperspectral system

- Use standard arc lamp for wavelength calibration



Post-processing for filter based systems

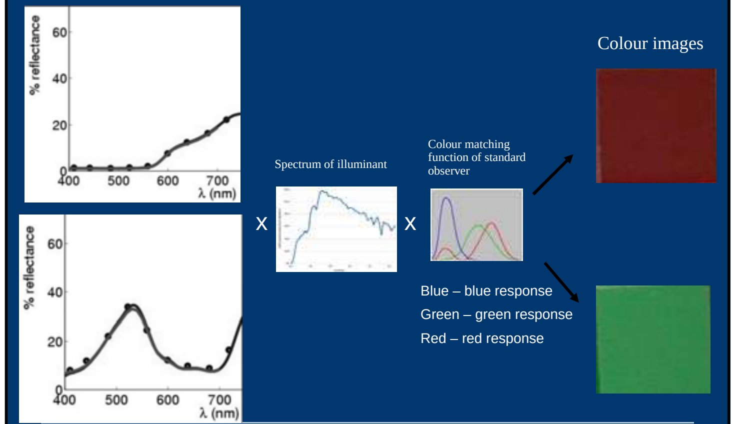
- calibration (dark subtract, flatfield, spectral calibration)
- alignment between channels
- mosaicing of individual images per channel
- For a given illuminant spectrum, calculate the colour image using the spectral reflectance
- Software packages:
  - Nip/VIPS free software (easy to use and designed for paintings/conservation) http://www.vips.ecs.soton.ac.uk
  - ENVI (remote sensing – very expensive; a huge package with lots of functions that are not needed for simple analysis)

Spectral imaging gives the following information for free:

- colour images
- Spectral reflectance per pixel
- Infrared images

400nm-880nm

Reflectance spectra & colour

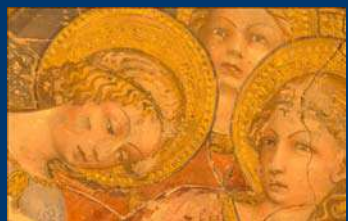


Rendering of colour images under different illuminant

Heads of Angels, wall painting fragment, National Gallery Collection

Daylight D65

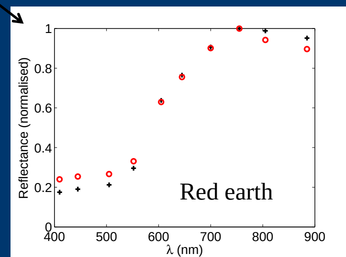
Candle light Illuminant A



Liang, Applied Physics A, 2012

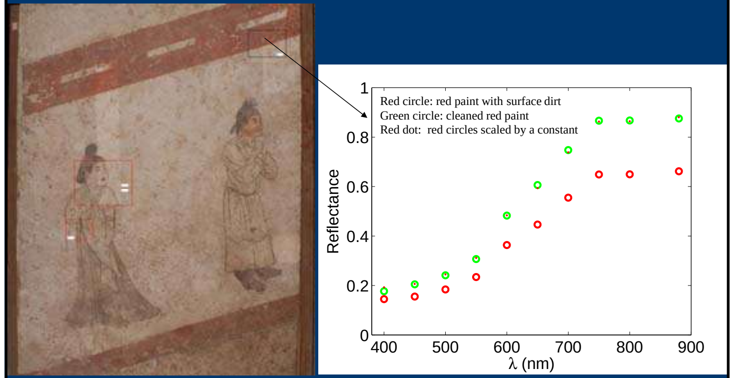
Pigment identification

Mogao cave 55 ceiling painting



Liang et al. ISPRS 2014

Effect of surface dirt

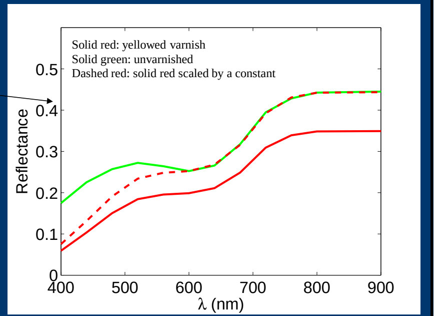


Tang dynasty tomb painting
Shaanxi history museum collection

Liang, Applied Physics A, 2012

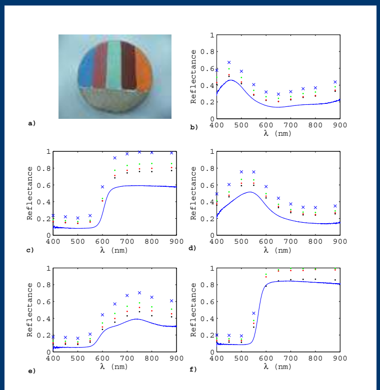
Effect of yellowed varnish

50 year old mastic varnish



Liang, Applied Physics A, 2012

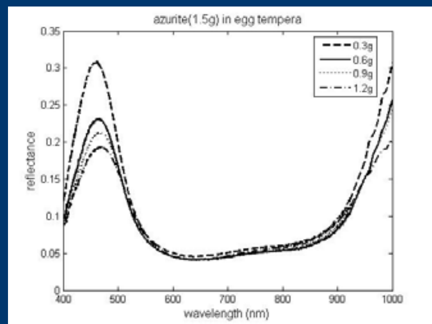
Effect of measurement geometry



Reflectance measured at various angles of incidence for a retro reflection geometry

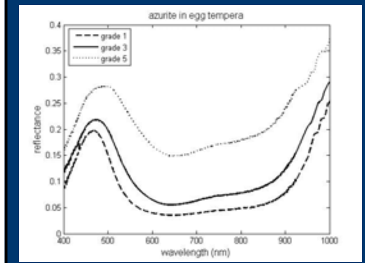
Liang et al., ISPRS Journal of Photogrammetry & Remote sensing, 2014

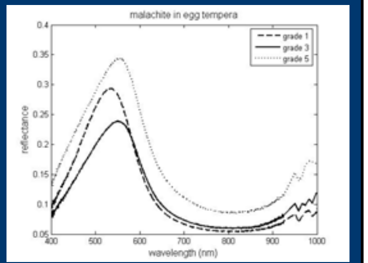
Effect of concentration



Effect of particle size

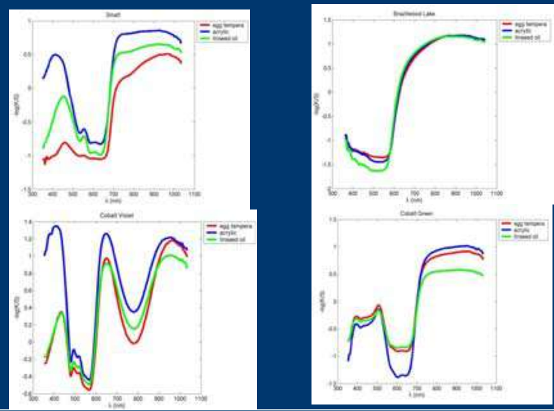
Increasing particle size from 5 to 1





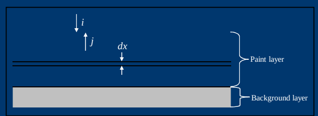
Liang et al. Applied Physics A, 2012 (review)

Effect of binding medium



Kubelka-Munk Theory

- For predicting the reflectance spectrum of a paint mixture – works well for highly scattering paints



$$-di = -(K+S)i\,dx + S\,j\,dx$$
$$dj = -(K+S)\,j\,dx + S\,i\,dx$$

If complete hiding $\frac{K}{S} = \frac{(1-R_\infty)^2}{2R_\infty}$

$$R = \frac{1 - R_g[a - b\coth(bSh)]}{a + b\coth(bSh) - R_g}$$

where $a = \frac{K+S}{S}$, $b = \sqrt{a^2 - 1}$

R_g – reflectance of background

K – effective absorption coefficient

S – effective scattering coefficients

h – thickness

Identification of pigment mixtures

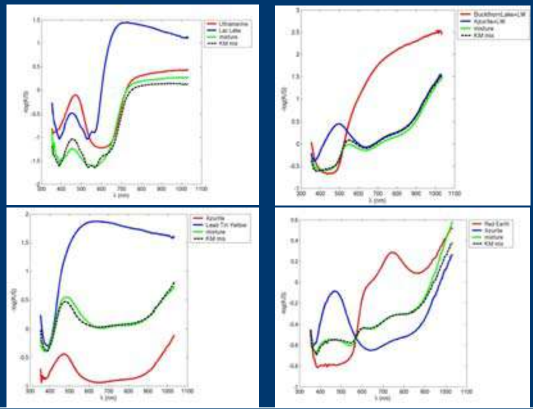
- It is possible to identify pigment mixtures using the spectral reflectance data and an algorithm that finds the concentrations c_1 and c_2 that gives the best fit to an unknown spectrum. The algorithm finds the combination of pigments that gives the best best fit spectrum. An educated guess as a starting point helps.

$$\left(\frac{K}{S}\right)_{tot} = c_1\left(\frac{K}{S}\right)_1 + c_2\left(\frac{K}{S}\right)_2 + \cdots$$

- Reflectance can be calculated from K/S
- Works best for highly scattering pigments, not so well for transparent and absorbing pigments

Liang, Applied Physics A, 2012

Mixing of pigments – Kubelka-Munk model can predict the spectrum of a mixture of two pigments



Imaging large areas at high resolution?

- Usual method: place the imaging system on a motorised scanner or painting on a motorised easel => still has a limit in maximum size

Multispectral scanner at the National Gallery London

Imaging wall painting on the ceiling?

- Usual method: place the imaging system on a scaffold platform
- Use a mechanical device to move the imaging system close to the ceiling

But we get high resolution images of the Moon from earth!

Design an imaging system that can give high resolution images from the ground as if it were within a metre of the object/painting.

Peterborough Cathedral nave ceiling (>30m from ground)

PRISMS (Portable Remote Imaging System for Multispectral Scanning)

- Visible range (400-900nm) : 10 filters
- d>3m telescope: D=90mm f=1250mm; d<3.5m lens: D=27mm f=150 mm
- Resolution: ~80 μm for distance of 10m

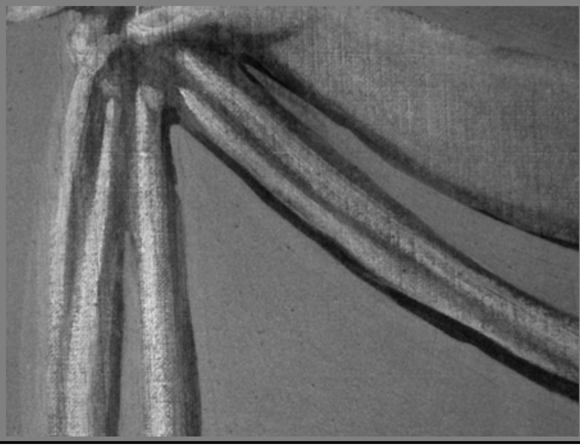
Liang et al., ISPRS Journal of Photogrammetry and Remote Sensing, 2014
Liang et al. SPIE, 2007

Modular PRISMS: A versatile spectral imaging system

PRISMS system developed at ISAAC can be used for remote spectral imaging of wall paintings and close range imaging of small objects in UV/VIS/NIR, SWIR

Kedleston Hall: imaging a painting in the Marble Hall at 23m
Photo taken by Stephen Boyd

Kedleston Hall: Marble Hall painting imaged from a distance of 23m at wavelength of 600nm



In situ imaging of paintings in gallery

- Simple setup – automatically scan any painting in the room from one central position
- No size limitation on the painting scanned

PRISMS in Nottingham Castle Museum

A 14th century wall painting in Byward Tower, Tower of London

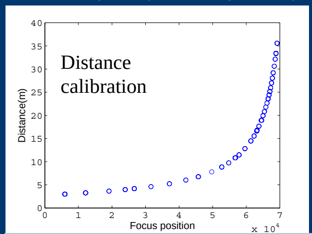
Automatic mosaicing of thousands of images

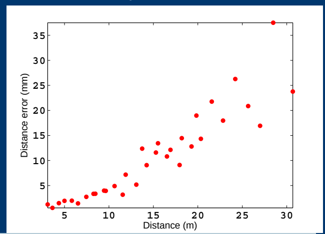
PRISMS for remote 3D topography

- *Position of focus is determined by the distance of the object*

=> distance measurement is a by-product of imaging (autofocus)
=> distance accuracy comparable to laser scanning

- *rms* distance accuracy ~5 mm at 10m distance for worst case scenario
- X-Y angular position given by motorised telescope drive





Liang et al. ISPRS, 2014

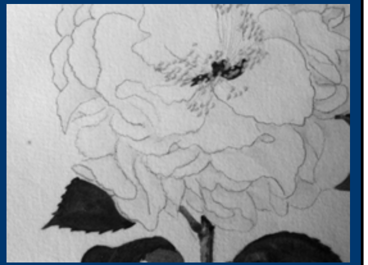
PRISMS: 3D spectral imaging all in one instrument

- Remote imaging – high resolution (~80 micron at 10m) imaging without scaffolding
- Close range imaging of small objects
- Fully automated capture & data processing
- Efficient in collecting spectral reflectance data
- Pigment identification
- Interband comparison to identify areas of alteration
- Reveal underdrawings and faded writings
- Accurate colour rendering under any illumination
- **Colour and 3D topography are by-products of spectral imaging => you get them for free!**

Liang et al., ISPRS Journal of Photogrammetry and Remote Sensing, 2014

Revealing underdrawing in NIR images

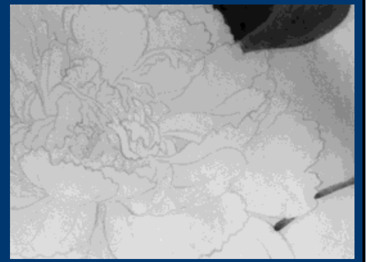
- Type of underdrawing: solid material



Multispectral imaging of paintings from the Reeves collection, Royal Horticultural Society

Revealing underdrawing in NIR images

- Type of underdrawing: ink

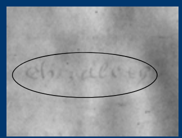


Multispectral imaging of paintings from the Reeves collection, Royal Horticultural Society

Kogou et al. Applied Physics A 2015

Revealing hidden writing using NIR, UV reflectance or UV fluorescence images

Prayer book, Bodleian Library, Oxford



Colour image

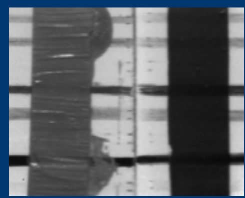
NIR 880nm image

Liang, BAR international series 2209, 2011

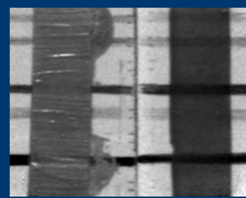
Colour, 1020, 1170, 1320, 1470, 1620nm (150nm bandwidth)

Dividing into narrower bands more likely to reveal underdrawings

- Azurite in linseed oil 50 microns thick (left)
- Prussian blue in linseed oil 100 microns thick (right)



900-1700nm



1620nm (150nm bandwidth)

Liang et al., IX CONGRESO NACIONAL DEL COLOR. ALICANTE 2010

4^{th} – 14^{th} century cultural exchange

– Buddhist cave temple paintings along the Silk Road

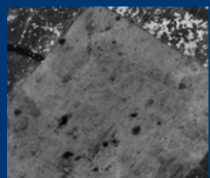
UNESCO world heritage site – Mogao caves near Dunhuang in the Gobi desert

UNESCO site in the Gobi desert – Mogao caves on the Silk Road (4^{th} – 14^{th} century)

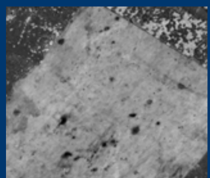
Liang et al. ISPRS, 2014

Revealing faded writing in Sanskrit on the ceiling automatically

Colour image



Visible 500 nm



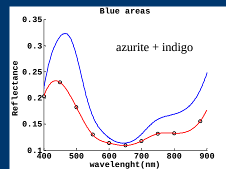
NIR 880 nm

Weighted subtraction
500 nm - 800 nm

Liang et al. ISPRS, 2014

The big data problem

- Auto-processing of data
  - Calibration, alignment
  - Mosaicing
  - Spectral => colour
  - Pigment & binder identification
  - Revealing ‘hidden’ features



PRISMS imaging the ceiling of cave 55 at 11-12m

Liang et al. ISPRS, 2014

High resolution remote imaging from 12m

Multispectral image cube => colour image for free

High resolution => green pigment particles visible from 12m

PRISMS imaging of cave 55 ceiling at 11-12m

Automatic mosaic of thousands of images

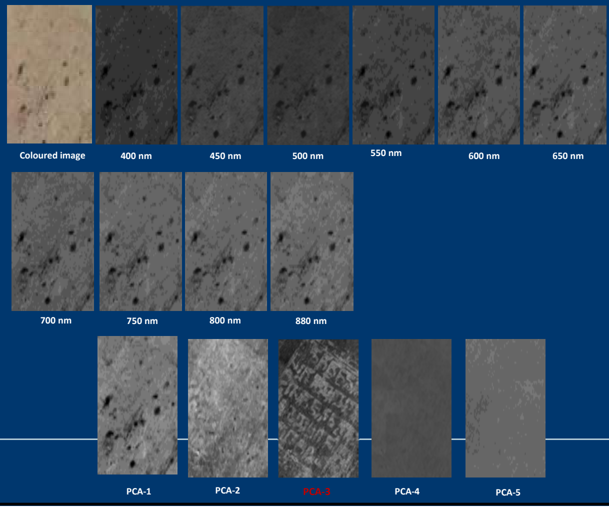
Liang et al. ISPRS, 2014

Statistical methods for spectral analysis

Multivariate statistics = Chemometrics

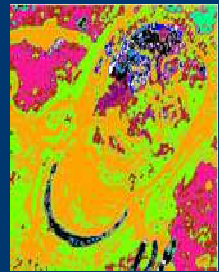
- Calculate Principle Component Analysis (PCA)
  - Components that are uncorrelated (or orthogonal to each other) based on maximizing variance
  - Calculate eigen vectors and eigen values of the correlation matrix
  - PCAs are calculated by applying the eigen vectors to the original bands of images
- Clustering of similar regions (many different methods), e.g. k-mean clustering (unsupervised technique) based on PCA scores to separate regions of similar spectral properties
- Software packages:
  - ENVI (remote sensing community – very expensive)
  - R free software but needs some programming ability

Automatic revealing of faded writings



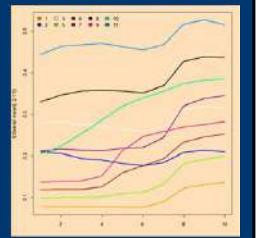
Spectral information combined with Statistical Analysis Methods

Coloured image derived form PRISMS image cube



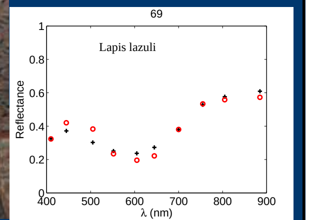
Spectral clustering of PRISMS image

Pigment classification using the **spectral information** derived from the PRISMS image cubes



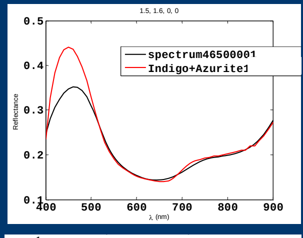
Material identification

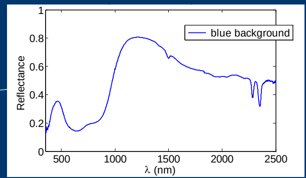
Dunhuang Cave 386 ceiling



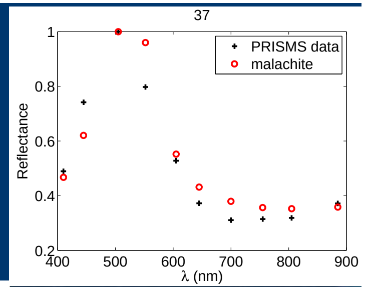
Identify combination of pigments

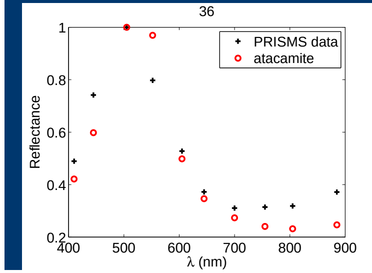
- Identify mixture using Kubelka-Munk theory => azurite, indigo

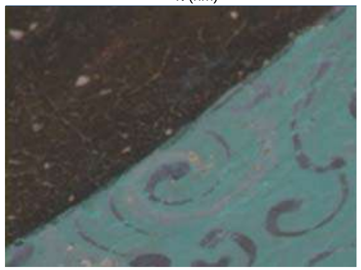




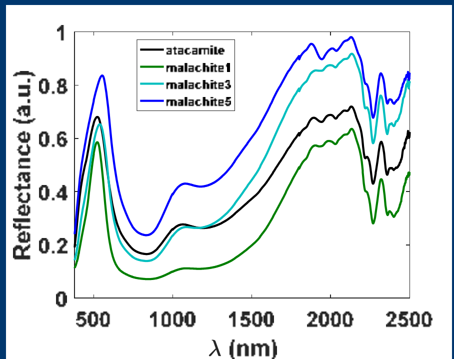
Comparison of normalized reflectance with malachite & atacamite reference spectra





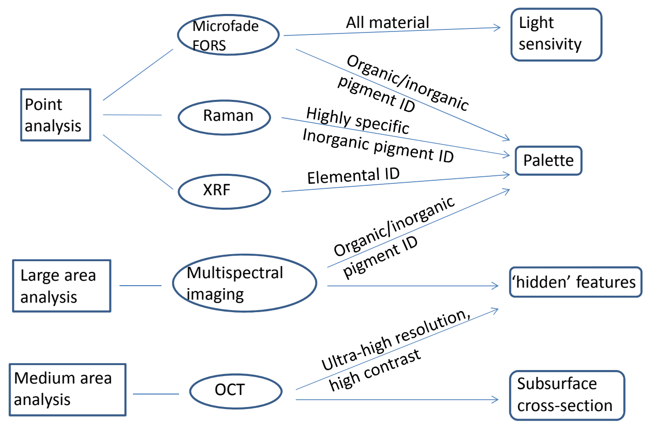


Malachite & Atacamite similar spectra (400-2500nm)



Atacamite spectrum compared with malachite of different particle size

A holistic approach to non-invasive investigation



Kogou et al. Applied Physics A, 2015

There is no Best techniques

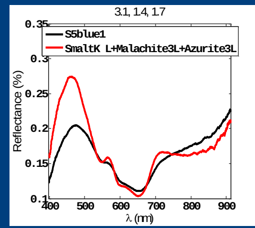
There are only complementary techniques
One technique cannot solve all problems

Technique	Working distance (mm)	Spatial resolution or spot size (mm)	Field of view or scanned size (mm)	Spectral range
Micro-Raman	~0.5	~0.002	~0.002	532 nm, 638 nm excitation, Raman shift range 150-3800 cm^{-1}
XRF	~1	~0.2	~0.2	2-50 keV
Microfade	~30	~0.46×0.76	~0.46×0.76	400-700 nm
VIS-NIR FORS	~30	~0.5	~0.5	400-950 nm
SWIR FORS	~2	~5	~ 5	900-2400 nm
UV-VIS-NIR spectral imaging	2240	~0.085	~115×85	400-900 nm
OCT	~10	~0.009×0.009×0.0045	~10 (width)	930 nm (100 nm bandwidth)

Kogou et al. Applied Physics A, 2015

Watercolour – an example (blueish region)

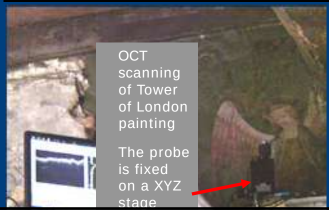
- Raman: azurite, malachite, goethite, unidentified blue crystal
- XRF: : Cu (Fe, Co, Pb, As) ((Mn, K, Ca))
- FORS: smalt, azurite, malachite
- => blue paint is a mixture of smalt, azurite, malachite (goethite is impurity of malachite)



Colour image derived from multispectral image, Chinese export painting, V&A collection

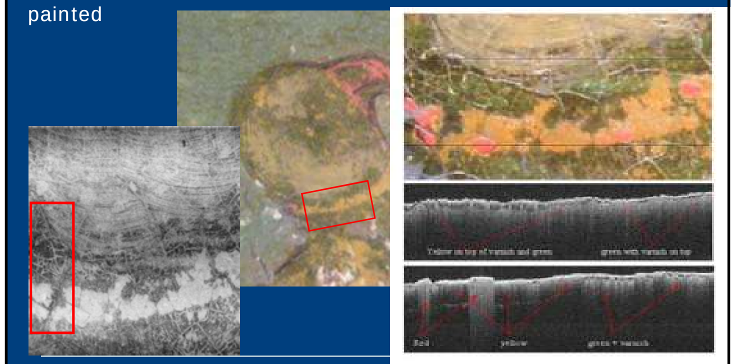
Kogou et al. Applied Physics A, 2015

Combined spectral Imaging & OCT Imaging of Wall Painting at Tower of London

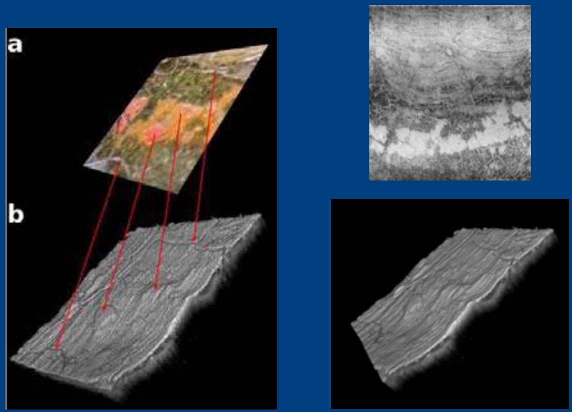


Areas of interest - popinjay

- The OCT data helps identify in which order parts of the bird were painted

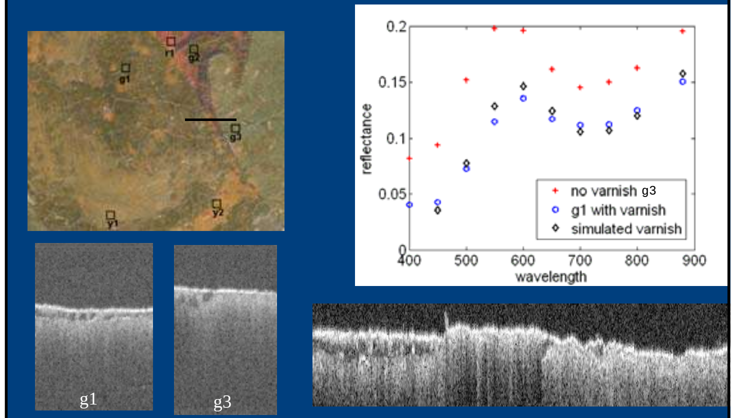


Liang et al. Proc. SPIE (2011) Vol. 8084, 80840F-1



Lange et al. SPIE Newsroom, August 2011

Virtual varnish removal



Liang et al. Proc. SPIE (2011) Vol. 8084, 80840F-1

Mobile instruments in ISAAC Laboratory – global access

Our unique in-house developed portable imaging and spectroscopy instruments for heritage science

Complementary commercial instruments

References

- Free download of full text for all the papers published by my group http://llr.ntu.ac.uk/rpd/researchpublications.php?pubid=18ea0ae3-8395-4d09-b763-637da94f532a or go to my web profile https://www.ntu.ac.uk/staff-profiles/science-technology/haida-liang and click on ‘go to Haida Liang’s publications’
- For all other relevant publications see references in my 2012 review article and citations to that review as well as references in our other later publications

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- The National Gallery (London): John Cupitt, David Saunders, Helen Howard & colleagues
- Victoria & Albert Museum: Lucia Burgio, Kate Bailey
- Royal Horticultural Society: Charlotte Brooks & colleagues
- Gooch & Housego plc: Chris Pannell, Jon Ward and colleagues
- Dunhuang Academy: Su Bomin and colleagues
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