FT-IR Spectroscopy

Agilent Technologies

600-IR Product line

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Agenda

Technology overview

Product line review

- Overview
- Instruments and Accessories

Markets and Applications

- Chemical analysis
- Life sciences

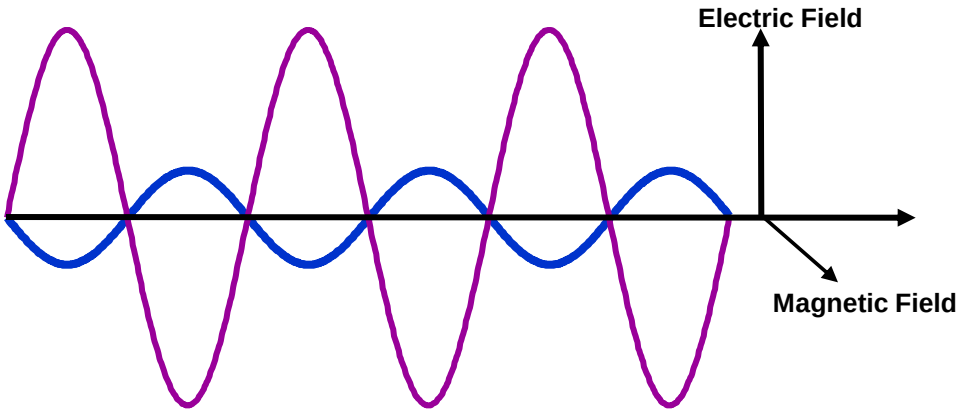
TECHNOLOGY OVERVIEW: BEGINNER'S GUIDE TO FT-IR SPECTROSCOPY

Part I

Basic concepts of FT-IR spectroscopy

Infrared spectroscopy (IR) is a powerful tool for the analysis of a wide array of samples.

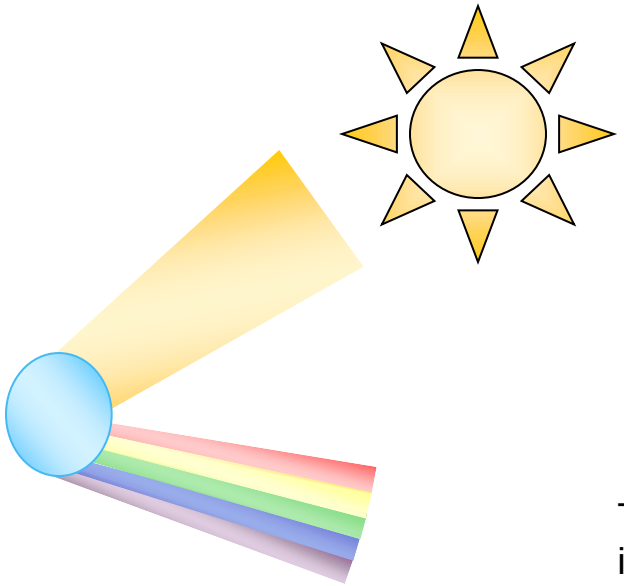
IR spectroscopy is the study of the interactions between infrared electromagnetic energy and matter, and allows for qualitative and quantitative measurements of samples.

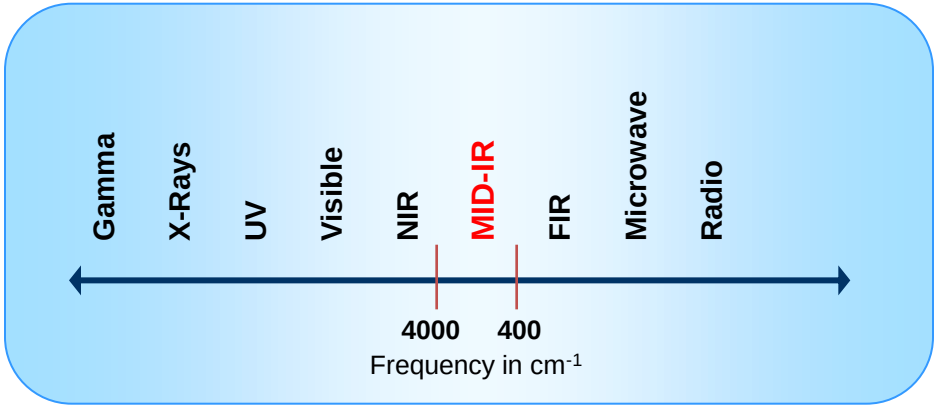


Technology

What is infrared light?

Infrared light is a portion of the electromagnetic spectrum, and is just beyond the visible portion of the spectrum





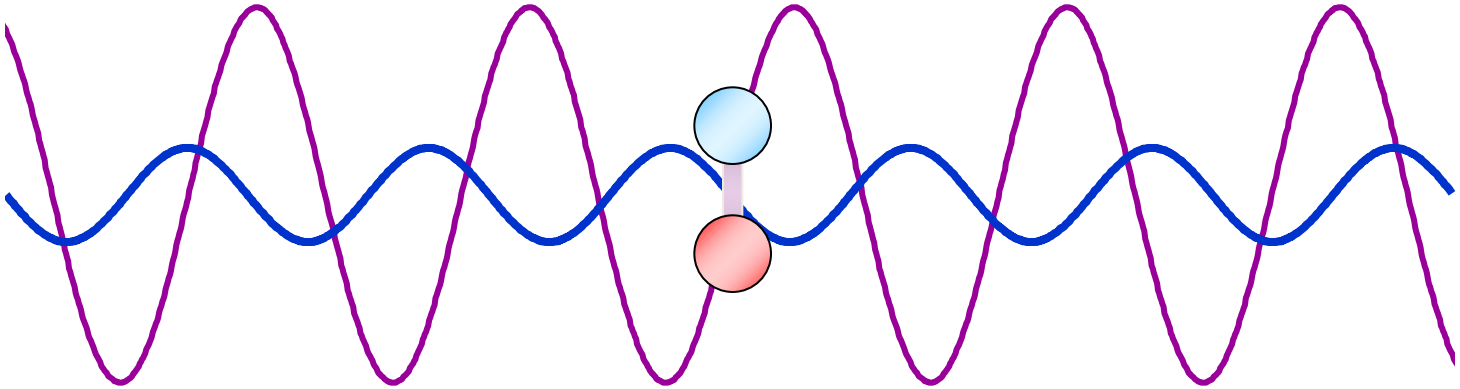
The electromagnetic spectrum can be divided into specific regions, including: Gamma rays, X-Rays, Ultraviolet, Visible, Infrared, Microwave and Radio.

For convenience of applications and instrumentation, the infrared spectrum is divided into near-, mid-, and far-infrared radiation. The most commonly used region is the mid-infrared.

Technology

Why can infrared light be used?

If infrared light energy is absorbed by a sample, it will cause an excitation of the sample's molecular vibrations.



This excitation causes the amplitude of chemical bonds to change. It is this change that is measured in infrared spectroscopy.

What can you measure with infrared light?

IR spectroscopy can be used to analyse samples from all three states of matter – it can be used to analyze **gasses**, **liquids**, and **solids**.

Infrared spectroscopy has been a cornerstone of analytical measurements for over 50 years.

Almost all compounds (whether they be organic or inorganic) absorb various portions of infrared light. Specifically, only chemical bonds that have a dipole moment that changes as a function of vibrations are capable of absorbing infrared light.

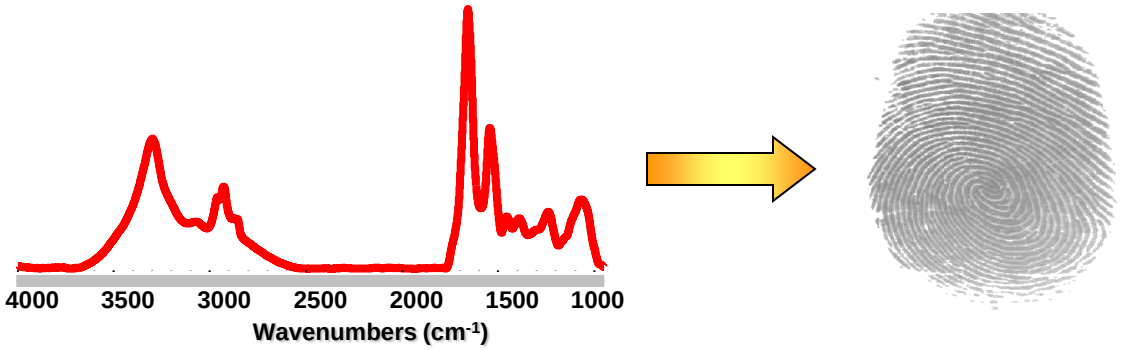
What is the basic principle of infrared spectroscopy?

- IR-active bonds produce peaks - Group frequency theory.

Bond	Type of Vibration		Wavenumber range (cm^{-1})
C—H	Alkane	(stretch)	3000 - 2850
	$-CH_3$	(bend)	1450 & 1375
	$-CH_2-$	(bend)	1465
	Alkene	(stretch)	3100 - 3000
		(out-of-plane bend)	1000 - 650
	Aromatic	(stretch)	3150 - 3050
		(out-of-plane bend)	900 - 600
	Alkyne	(stretch)	~3300
	Aldehyde		2900 - 2700
C═C	Alkene		1680 - 1600
	Aromatic		1600 & 1475
C≡C	Alkyne		2250 - 2100
C═O	Aldehyde		1740 - 1720
	Ketone		1725 - 1705
	Carboxylic acid		1725 - 1700
	Ester		1750 - 1730
	Amide		1680 - 1630
	Anhydride		1810 & 1760
C—O	Alcohols, esters, ethers, carboxylic acids, anhydrides		1300 - 1000
O—H	Alcohols, phenols		
	Free		3650 - 3600
	H-Bonded		3400 - 3200
	Carboxylic acids		3400 - 2400
N—H	Primary and secondary amines & amides		
		(stretch)	3500 - 3100
		(bend)	1640 - 1550
C—N	Amines		1350 - 1000
C═N	Imines and oximes		1690 - 1640

What is the basic principle of infrared spectroscopy?

- IR-active bonds produce peaks - Group frequency theory.
- Every different type of chemical bond that absorbs infrared light naturally vibrates at a specific frequency.
- Small variations result in peak position and height allow for differentiation.
- IR spectrum can serve as a compound's fingerprint.



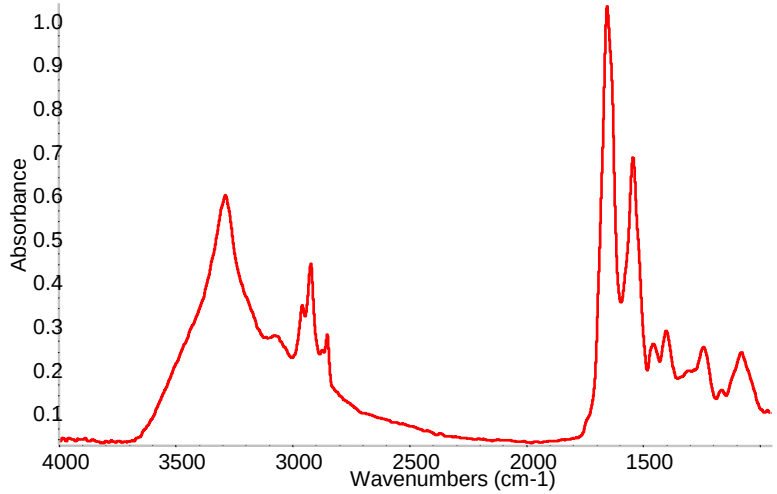
Why use FT-IR spectroscopy for analytical measurements?

- FT-IR analysis is SIMPLE to perform
- FT-IR provides incredibly ACCURATE results
- Results are available within SECONDS to MINUTES
- The method is VERSATILE
  (can accommodate various sample sizes and types)
- Powerful tool for analysis of any GAS, LIQUID or SOLID
- Provides both QUANTITATIVE and QUALITATIVE results
- FT-IR analysis CAN BE NON-DESTRUCTIVE
- FT-IR spectroscopy is an AFFORDABLE method
- FT-IR can require very little to NO SAMPLE preparation

How can FT-IR spectroscopy help me?

- FT-IR spectrometers are ideal for routine QA/QC analyses. Their use ranges from very simple analyses, to very complex and informative nanosecond time-resolved experiments.

- FT-IR is application based – it helps to have a basic understanding of the scope of applications in order to feel comfortable discussing how it can solve analytical problems.



Technology

What fields can FT-IR spectroscopy be applied to?

FT-IR spectroscopy is routinely used in:

- Biosciences
- Polymers
- Food & Agriculture
- Environmental Analysis
- Material Sciences
- Pharmaceuticals
- Forensics
- Chemical Analysis
- Fuels and Energy

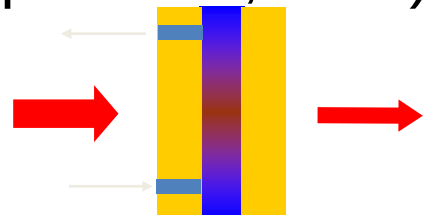
It offers affordable performance in all of the above listed areas, sample identification, verification, and education.

This tool provides performance, flexibility, and upgradeability for demanding QA/QC tasks, as well as product development, troubleshooting, and applied research & development.

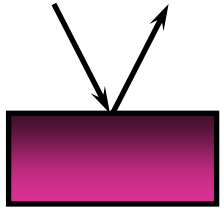
Technology

FTIR Sampling Modes

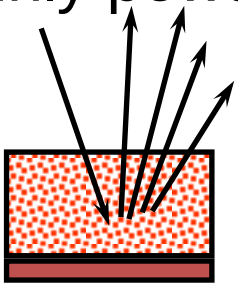
Transmission
(liquids, gases, powders, films)



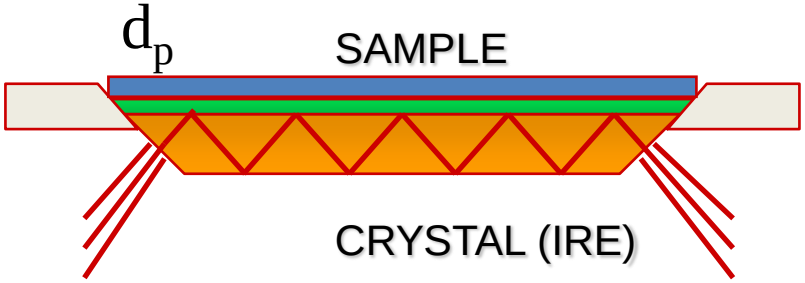
Reflectance
(liquids, thins films, shiny bulk materials)



Diffuse Reflectance
(mainly powders)

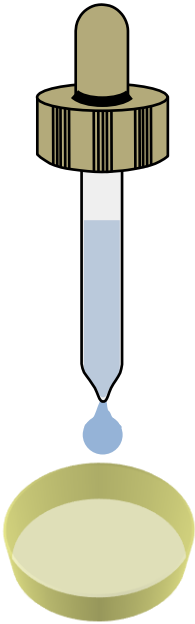


ATR (Attenuated Total Reflectance)
(all, except gases)



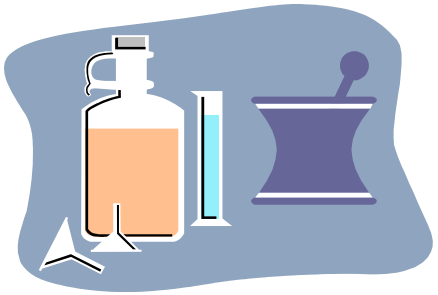
Transmission: Sample Preparation for IR

- Cast Films - for solid powders and polymers and non volatile solvents
  - Dissolve in a volatile solvent or melt.
  - Apply liquid to an infrared transparent window, allow to dry/solidify.
  - With luck and skill, could get film neither too thick nor too thin, without excessive baseline tilt from crystalline scattering, without cracking or flaking off the window, which would produce a good spectrum.



Transmission: Mulls

- Mulls - For powders which could not be dissolved, or would not melt and flow.
  - Sample ground in a agate mortar with a *Mulling Agent*.
  - Mulled sample applied to pair of infrared windows as a capillary film.
  - With skill and luck, could get a mull that was not too thin or thick, properly ground, and did not react with mulling agent or windows.
  - Different mulling agents required to get a complete infrared spectrum (all absorb in the IR and interfere in different regions of the spectrum.)



Transmission: Pressed Pellets

For solids and powders.

- Sample ground “talcum powder fine”, mixed with finely ground NaCl or KBr powder at ~1% w/w sample/salt.
- Salt must be absolutely dry.
- Salt may react with sample (ion exchange).
- Mixture placed in die, compressed under several tons of pressure to form an infrared transparent pellet.
- With skill and luck, a clear pellet that was not too thick or thin, and not cloudy or hazy (from large sample particles) would be formed.

Transmission: Gas Analysis

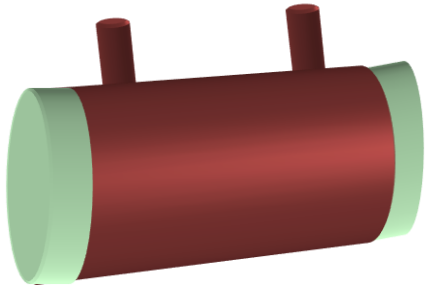
- Gases much weaker infrared absorbers, use longer pathlength to increase absorbance signal intensity.

  Typical gas cells:

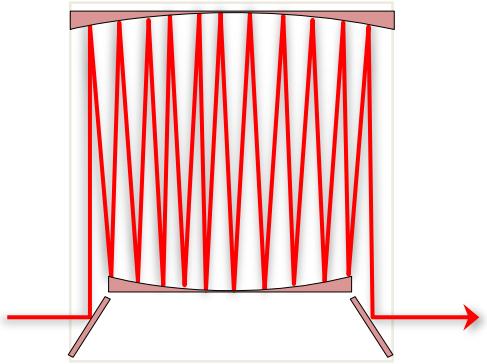
  - 10 cm single-pass.
  - Multi-pass gas cells.

  Windows, mirrors (in multi-pass cells), cell body and fittings must be compatible with sample.

  Environmental applications use “open-air” or “fence-line” techniques.



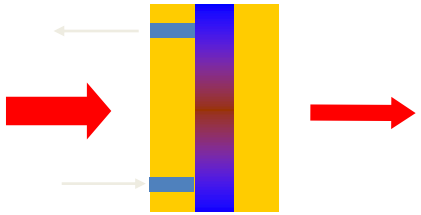
10 cm Gas Cell



Multi-pass Gas Cell

Transmission: Liquid Cells (mainly for quantitative analysis)

- Two infrared transparent windows, separated by a metal or polymer (typ. PTFE) spacer, 0.05 to 1 mm path length.



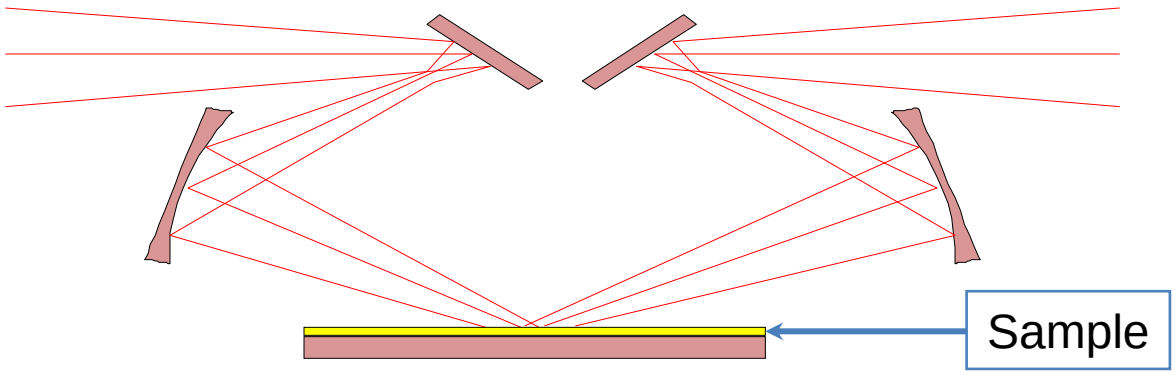
Cell Types:

- “Demountable”, two windows and assorted spacers that can be interchanged.
- “Sealed Amalgam”, windows sealed with lead-amalgam spacer, can not be disassembled.
- Variable-Path, two fixed windows in threaded sleeve.

High-pressure, high-temperature configurations are also available.

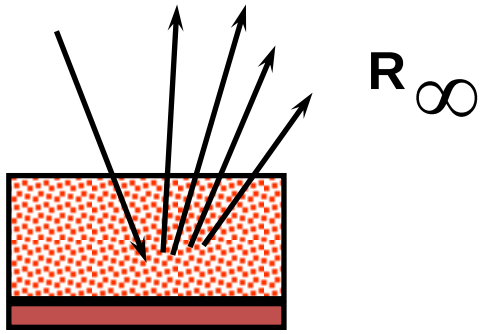
Reflectance: Specular Reflectance

- For thin coatings on reflective surfaces, also for bulk polymers (qualitative only).
  - Angle of incidence and collection varied, shallower angles increasing pathlength through the organic coating (grazing-angle reflectance).



Diffuse Reflectance (DRIFT)

- For powders and other finely ground material.
  - Sample ground, mixed with salt (KBr) in same proportions as for pressed pellet.
  - Mixture placed in DRIFT cup, infrared spectrum acquired, using pure KBr in another sample cup as the background.
  - Common technique for Sampling in the Near Infrared, e.g., solid tablets
  - Response depends on
    - particle size (smaller stronger)
    - packing (tighter less diffuse)
    - dilution often important (concentration ~1%)

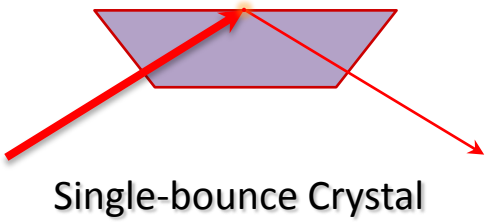


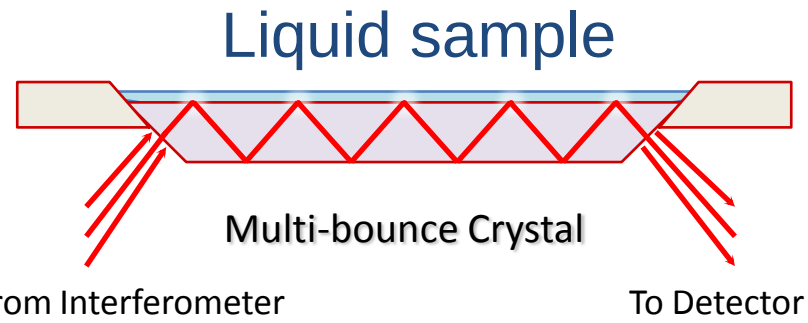
Attenuated Total Reflectance (ATR)

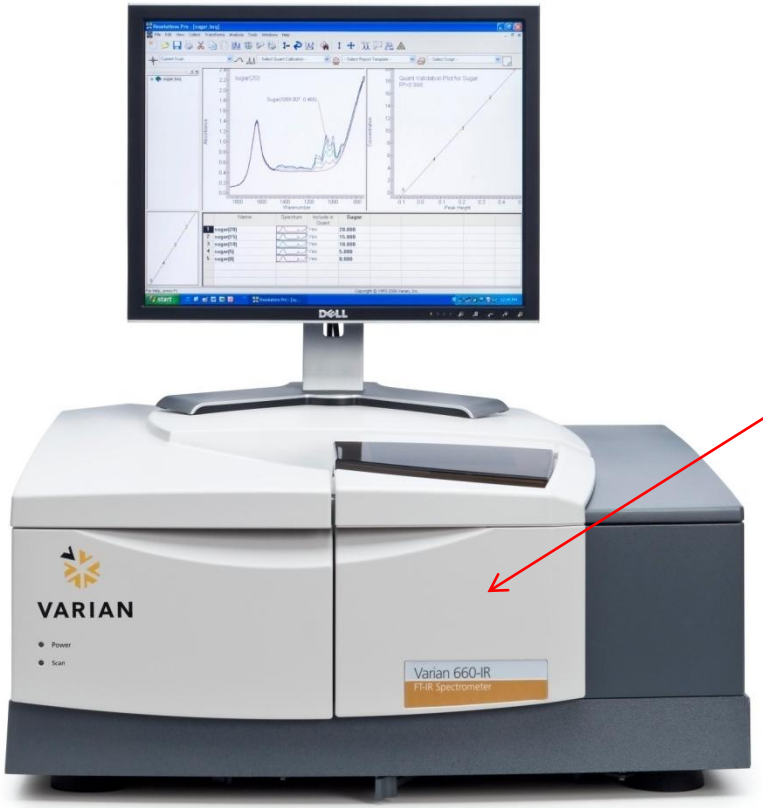
For liquids (organic & aqueous) and solids, especially polymers.

•Infrared beam internally reflects through the crystal, interacting with sample in contact with the crystal surface.

•Surface effect wavelength dependent, shorter wavelengths (higher wavenumbers) interact less.







Confirm consistency

600-IR PRODUCT LINE REVIEW

A. Overview

B. Instruments and Accessories

Part II

In a class of their own…

A combination of Agilent's (through Varian) 60 years of Molecular Spectroscopy experience with over 40 years of Digilab FT-IR innovation has resulted in a new era in FT-IR spectroscopy

Introducing the Agilent 600-IR Series

- A range of FT-IR spectrometers, from routine to research, targeting a wide range of markets, customers and their applications
- Microscope and Chemical Imaging solutions that extend your spectrometer beyond traditional use

A History of Spectrometer FIRSTS

A History of Commercial 'Firsts'

The Varian 660/670/680-IR series is the culmination of 40 years of Digilab's FT-IR technology acquired by Varian, enhanced with 60 years of Varian's own molecular spectroscopy expertise. Incorporating many FT-IR commercial 'firsts', you can be assured that your FT-IR stems from a formidable history of innovation and excellence.

- First commercial FT-IR spectrometer.
- First use of a mercury cadmium telluride (MCT) detector in an FT-IR.
- First FT-IR microscope.
- First dynamically aligned step-scan interferometer.
- Patented linearized MCT detector[1].
- Patented digital signal processing software for photoacoustic spectroscopy (DSP1™)[2], polymer stretching (DSP2™)[3] and polarization modulation (DSP3™)[4] experiments.

[1] United States Patent 5,262,635. [2] United States Patent 5,612,784.
[3] United States Patent 6,020,962. [4] United States Patent 6,025,913.

And many more…

A History of Microscope FIRSTS

A History of Commercial 'Firsts'

The Varian 610/620-IR microscope series is the culmination of 40 years of Digilab's FT-IR technology acquired by Varian, enhanced with 60 years of Varian's own molecular spectroscopy expertise. Incorporating many FT-IR commercial 'firsts', you can be assured that your FT-IR stems from a formidable history of innovation and excellence.

- First commercial FT-IR spectrometer
- First FT-IR microscope
- First infinity-corrected FT-IR microscope
- First near-IR array detector system for spectroscopy imaging
- First mid-IR FPA[1] detector system for chemical imaging
- First rapid-scanning FPA[1] chemical imaging system
- First ATR chemical imaging system[3]
- First large sample microscope objective[2]

[1]Export of this product is regulated by the U.S. Department of State in accordance with guidelines of the ITAR per Title 22, CFR, Parts 120-130

[2]United States Patent 6,661,573

[3]United States Patent 6,141,100; British Patent GB 2329977; German Patent DE 198 36 758;

And many more…

Overview

Important Performance Specifications

- Signal-to-Noise (SNR) = sensitivity
- Spectral Resolution
- Spectral Range (UV, Vis, Near-IR, Mid-IR, Far-IR)
- Speed (spectra/sec) – kinetic measurements

The current (and potential future) application needs will define which specifications are most important

FT-IR product line overview - Spectrometer

Agilent 640-IR

Entry-level to Midrange

Routine measurements
QA / QC
Academic Teaching

Agilent 660-IR

Midrange

Routine measurements
QA / QC
Academic Teaching
Method Development
Research

Agilent 670-IR

Mid - High End

Method Development
Applied & Fundamental Research
Hard-to-analyze samples

Agilent 680-IR

High end

Fundamental Research
Hard-to-analyze samples

UPGRADABLE

Agilent 640-IR Specifications

Parameter	Agilent 640
SNR (1 min)	>28,000:1
SNR (5 sec)	>8,000:1
SNR (ATR, 5 sec)	>2,300:1
Speed (scans per sec)	> 40
Spectral coverage range	14,800 – 225 cm^{-1} Fixed: either MIR or NIR
Energy Throughput at sample	> 35 mW
Resolution (unapodized)	0.18 cm^{-1}
Wavenumber accuracy	>0.01 cm-1
Wavenumber precision	>0.005 cm-1

Why is this SNR good, and why does a customer care?

This SNR means that a user can see analytes and components that would otherwise not be visible with other FT-IRs.

Why is Max Kinetics Speed good?

Allows users to investigate faster reactions. This scan speed is better than all competitors, and provides more detailed kinetic information.

Incredible sensitivity & Ease of Use

Instruments

Agilent 660 / 670 / 680-IR Spectrometers

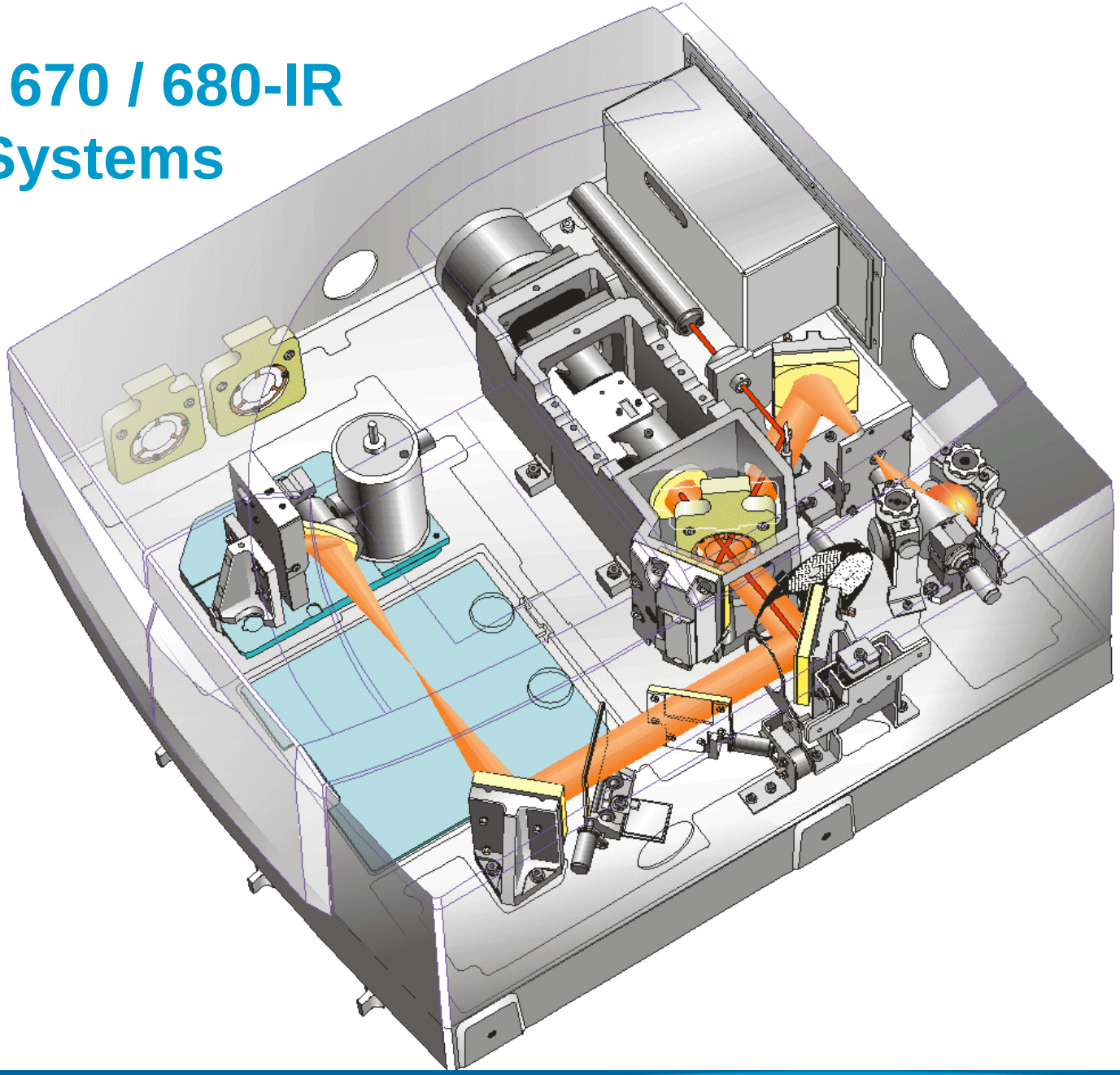
Agilent 660

Agilent 670

Agilent 680

Instruments

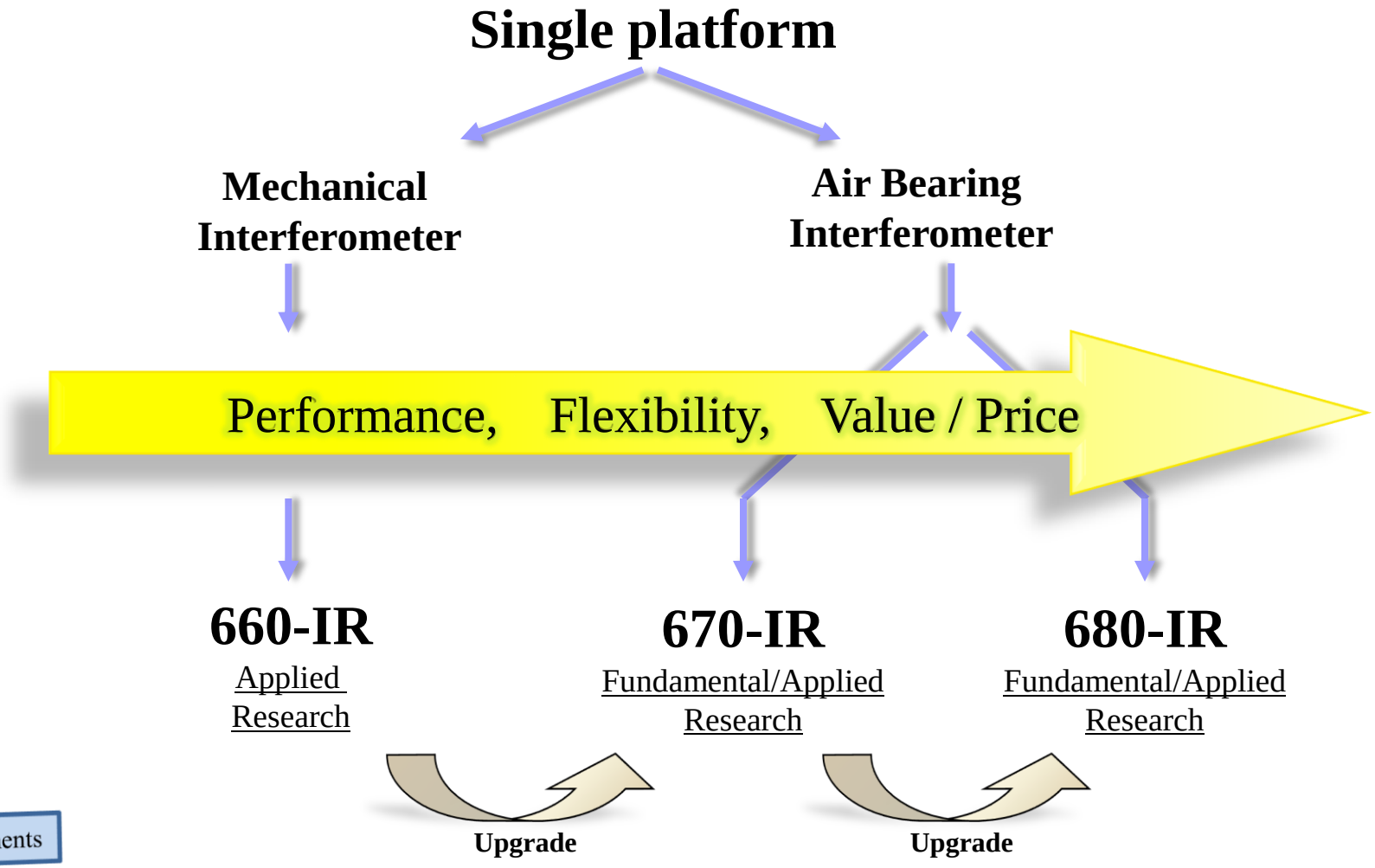
660 / 670 / 680-IR Systems



Instruments

Upgradeability Path Between 660 / 670 / 680-IR Systems

Ability to Upgrade = Growing with your research; "*Future Proof*"



Agilent 660-IR Spectrometer

- Provides better resolution, performance, & flexibility than competitors within and above its class.
- Ideal for applied research & development, product development, as well as troubleshooting, and QA / QC applications
- Upgradeability from Mechanical to Air Bearing

Applied research instrument that has been customized for users who wish to conduct more demanding experiments in less time with greater accuracy.

Instruments

Agilent 660-IR Specifications

Parameter	Agilent 660
SNR (1 min)	>50,000:1
SNR (5 sec)	>16,000:1
SNR (ATR, 5 sec)	>4,500:1
Speed (scans per sec)	> 65
Spectral coverage range	50,000 – 20 cm^{-1}
Energy Throughput at sample	> 50 mW
Resolution (unapodized)	>0.075 cm^{-1}
Wavenumber accuracy	>0.005 cm-1
Wavenumber precision	>0.003 cm-1
Upgradeable	YES
Dual Source/Det. Option	YES
Interferometer	**Mechanical**
External Source Option	NO

Instruments

Why is this spectral range good, and why does a customer care?

This spectral coverage range is great because it allows the customer to choose between performing UV-Vis, Near-IR, Mid-IR, or Far-IR experiments on the same system.

Why is this resolution good?

This unapodized resolution means that our customers can better characterize their samples and differentiate peaks that are close to each other *(esp. for gases)*.

Data sheets & proof statements are available to support claims

Agilent 670-IR & 680-IR Spectrometers

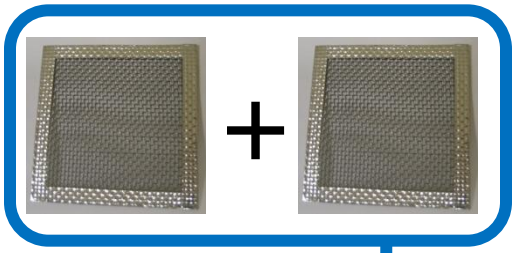
- Tailored to Fundamental Research - Deliver massive energy throughput, and Better SNR than ANY other spectrometer in the world
- Optimized for applications with attenuating accessories (ATR, Microscopy, Imaging, IGG)
- Innovative design of spectrometers no longer requires H_2O cooled source
- The Agilent 670-IR & 680-IR offer maximum versatility, deliver unsurpassed speed and higher sampling sensitivity

Advanced research instruments that deliver more infrared energy than any instrument in the market.

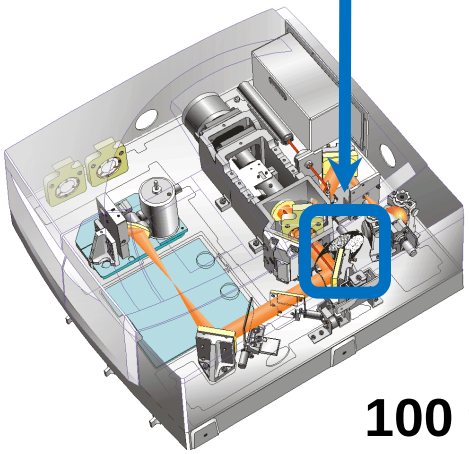
Instruments

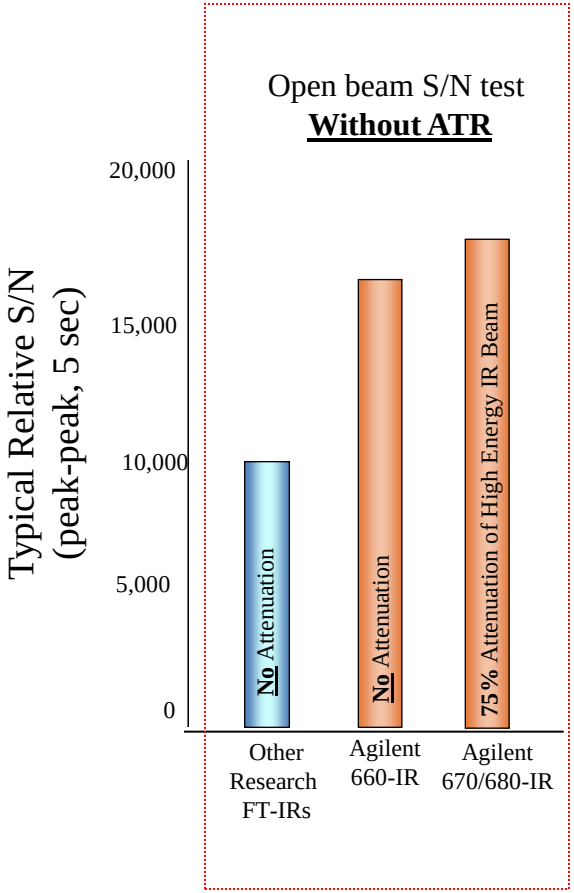
Agilent 670/680-IR SNR Comparison

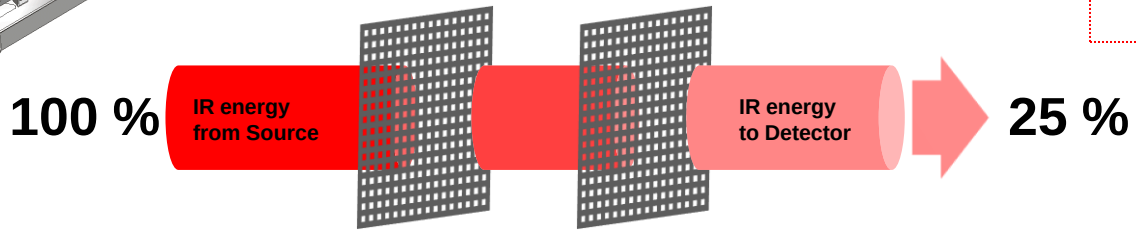
= 50 % beam attenuation.
This means that only ½ of IR energy reaches the detector.



= 75 % beam attenuation.
This means that only ¼ of IR energy reaches the detector.







Agilent 670-IR & 680-IR SNR Comparison

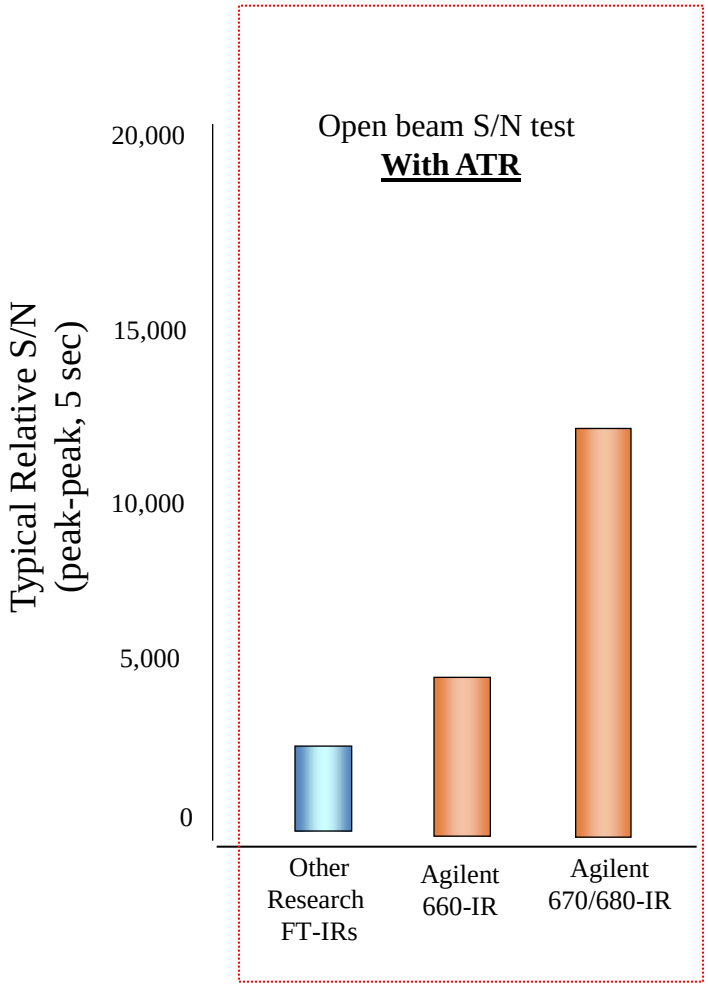
ATR accessories **cause**
75 to 90 % beam attenuation

+

≈

Addition of ATR

(80% attenuation)



Why does a customer care?

- ATR is EASY for sampling
- This performance means faster collection
- More importantly, this means they can detect lower concentrations of sample

Instruments

Agilent 670-IR & 680-IR Specifications

Parameter	Agilent 670/680
SNR (1 min)	>50,000:1 **WITH 75% ATT**
SNR (5 sec)	>17,500:1 **WITH 75% ATT**
SNR (ATR, 5 sec)	>12,000:1
Speed (scans per sec)	> 110
Spectral coverage range	50,000 – 10 cm^{-1}
Energy Throughput at sample	> 160 mW
Resolution (unapodized)	>0.075 cm^{-1}
Wavenumber accuracy	>0.005 cm-1
Wavenumber precision	>0.003 cm-1
Upgradeable	YES
Dual Source/Det. Option	YES
Interferometer	Air
External Source Option	Yes

Instruments

Why is this SNR good?

This SNR is UNPRECEDENTED. ['With ≥75% beam attenuation' means that only 25% of IR energy is used.] This means that when a customer analyzes a sample with an accessory (ATR, Microscope, Imaging), they will obtain unparalleled SNR.

Why is this spectral range good?

It allows for UV-Vis, Near-IR, Mid-IR, or Far-IR experiments on the same spectrometer. This means that a customer can analyze any sample that they want with ease.

Why is this energy throughput good?

More IR energy at the sample means that 'hard-to-analyze' samples become 'easy'.

Advanced Spectrometer Options

Parameter	
Step-Scan	Step-scan data collection is appropriate for many time-dependent measurements.
Time Resolved Spectroscopy *	A customer can monitor the progress of reproducible reactions or spectroscopic processes on a micro to nanosecond scale.
PM-IRRAS *	Allows for the sensitive measurement of monolayers and their molecular orientation.
Photoacoustic depth profiling *	Provides information from multiple layers of depth simultaneously with NO sample prep.
Polymer Stretching *	Practical means of studying molecular orientation and stress-strain measurements.

*** Requires the purchase of additional hardware**

Agilent 660/670/680-IR Spectrometer Options

Parameter	Agilent 660	Agilent 670	Agilent 680
Step-Scan	Upgrade	Upgrade	YES
Time Resolved[1] Spectroscopy	Upgrade	Upgrade	YES
PM-IRRAS[2]	YES	YES	YES
Photoacoustic depth profiling	YES	YES	YES
Polymer Stretching[1]	Upgrade	Upgrade	YES

1. Requires Step Scan (680 Only)

2. Requirs Dual A/D option for 660

The Agilent 680 has all the components of the 670 with ADDITIONAL capabilities

AGILENT 610 / 620-IR MICROSCOPE

Agilent 610 / 620-IR Microscope

Agilent 610-IR Microscope

Single Element & Dual Single Element

Agilent 620-IR Microscope

Infrared Imaging & Single Element

Instruments

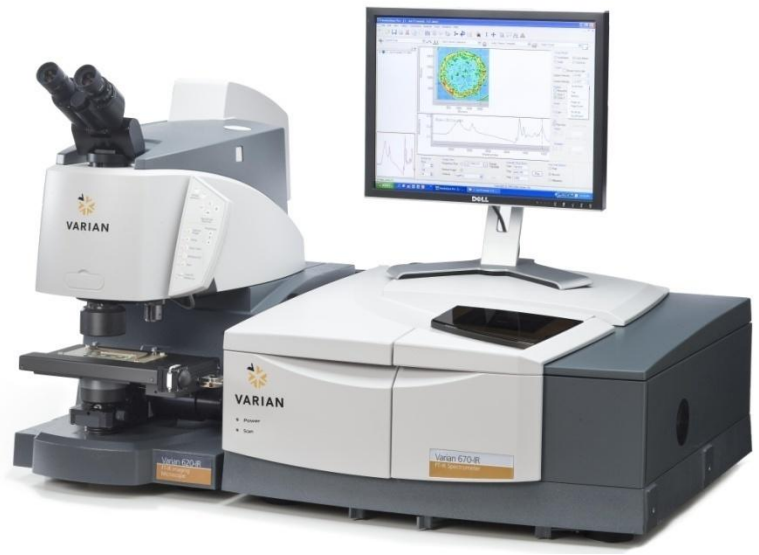
What is an Infrared Microscope

An Infrared microscope purposes:

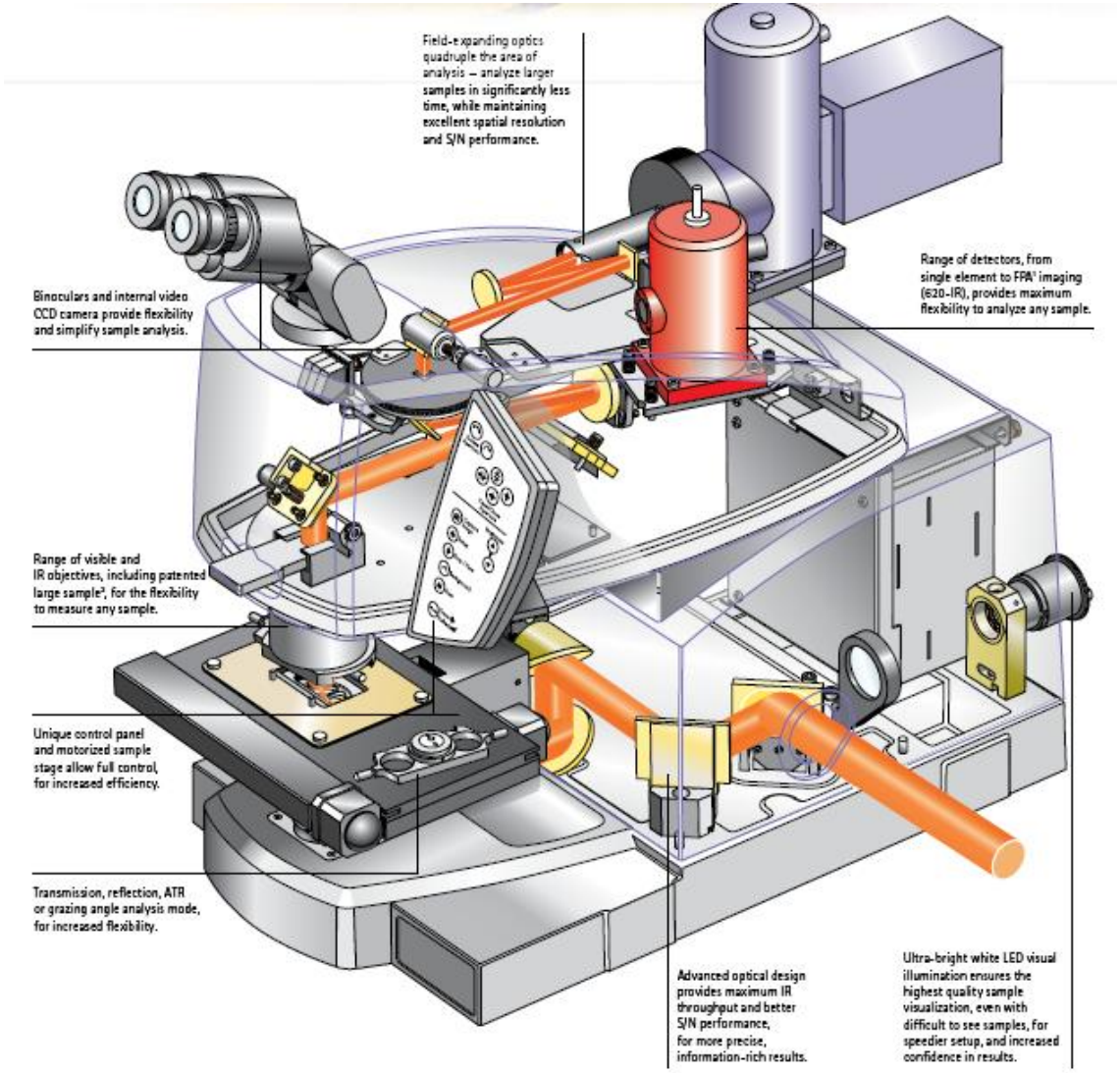
- To allow the user to see small (micron sized) samples
- To obtain accurate infrared spectra on those small samples

Infrared microspectroscopy can be done in three modes:

- Single point
- Mapping
  - Single point
  - Linear Array
- 2-D Focal Plane Array (FPA) Imaging



Improved Optical and Hardware design

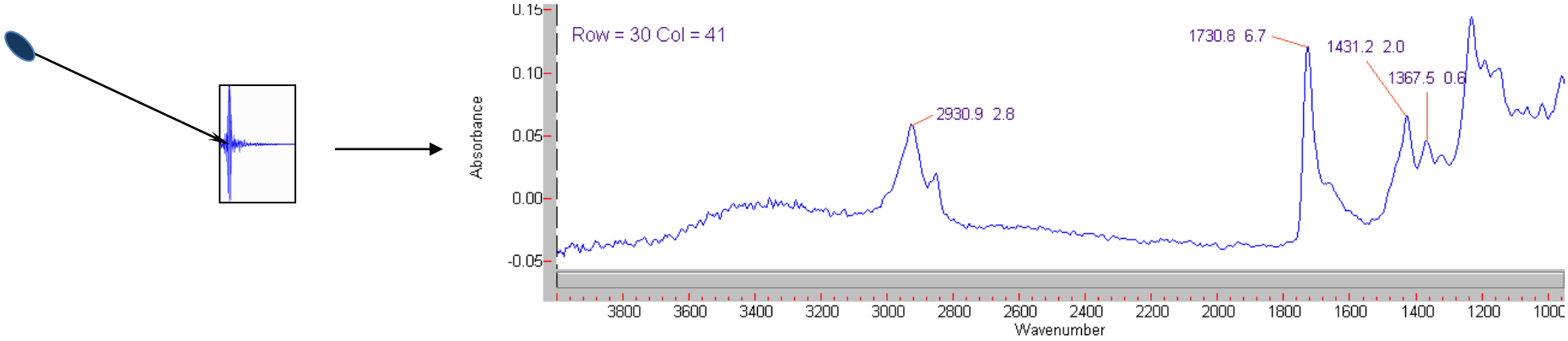


Single point analysis

(Single-element detector analysis)

Single Point Analysis

1 detector element collects 1 spectrum per scan



Desired spatial resolution is attained by fixing aperture size to desired sampling size. This eliminates spectral interference from the surrounding area.

Typical achievable spatial resolution is 10 - 20 µm.

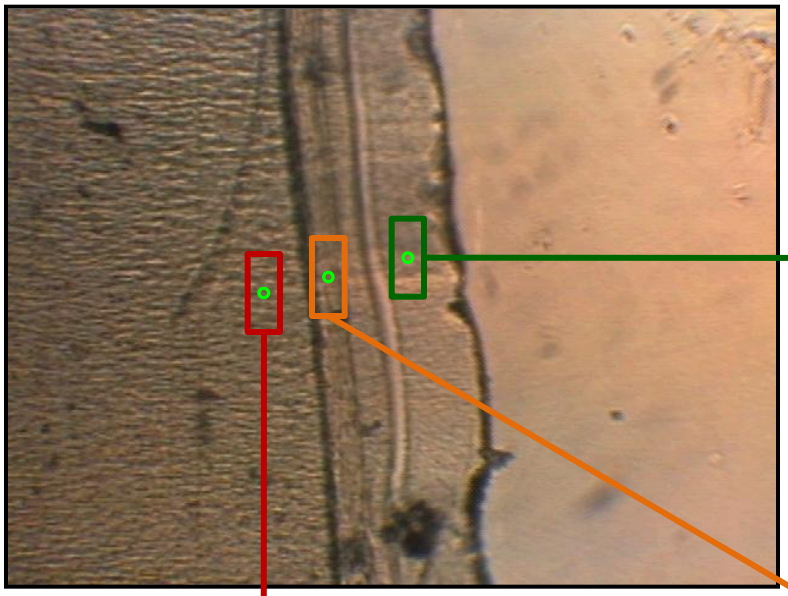
Basic Experiments

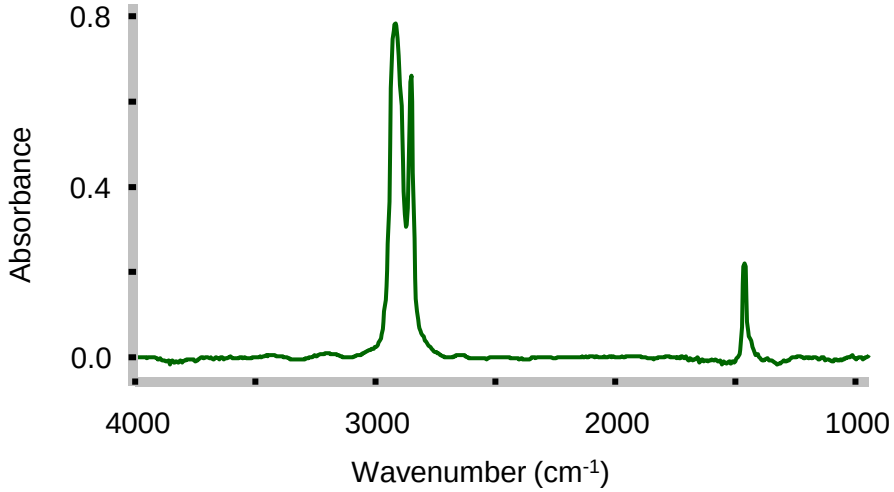
Transmission

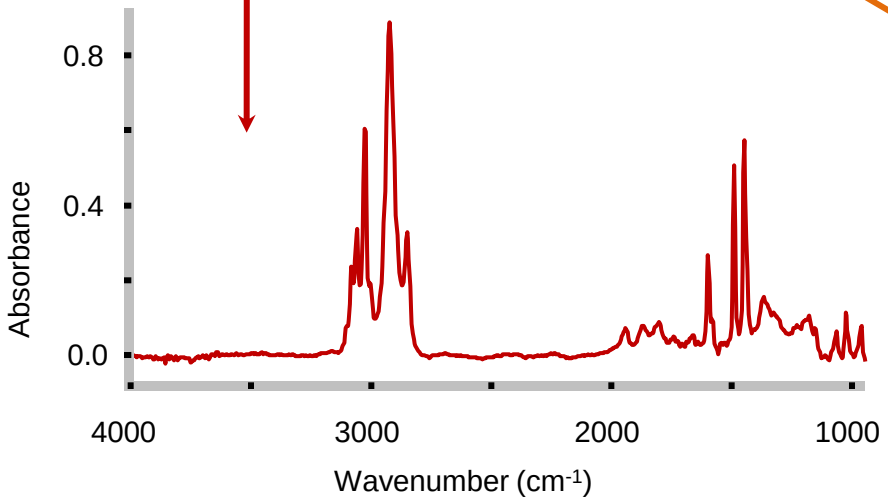
Reflection

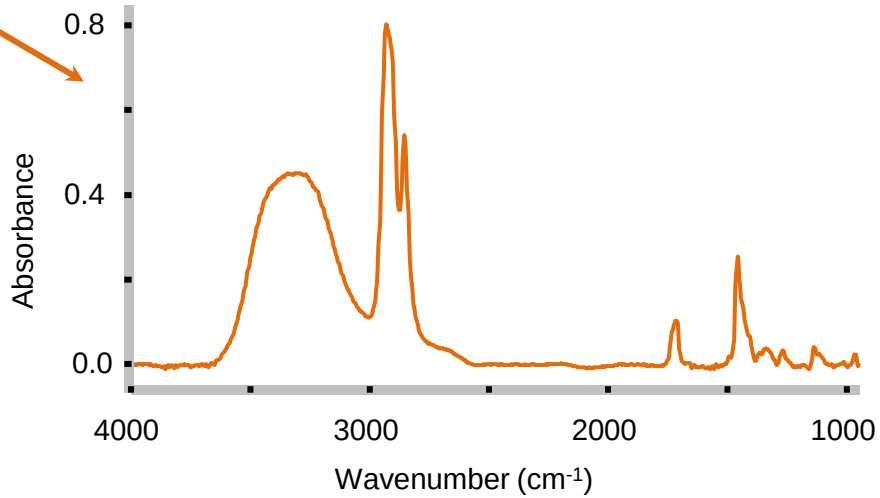
- Reflection Absorption
  - Near normal incidence
  - Grazing angle incidence
- Specular reflection
- Diffuse reflection
- Attenuated total reflection (ATR)

Transmission IR Analysis of Microtomed 3 layer Laminate

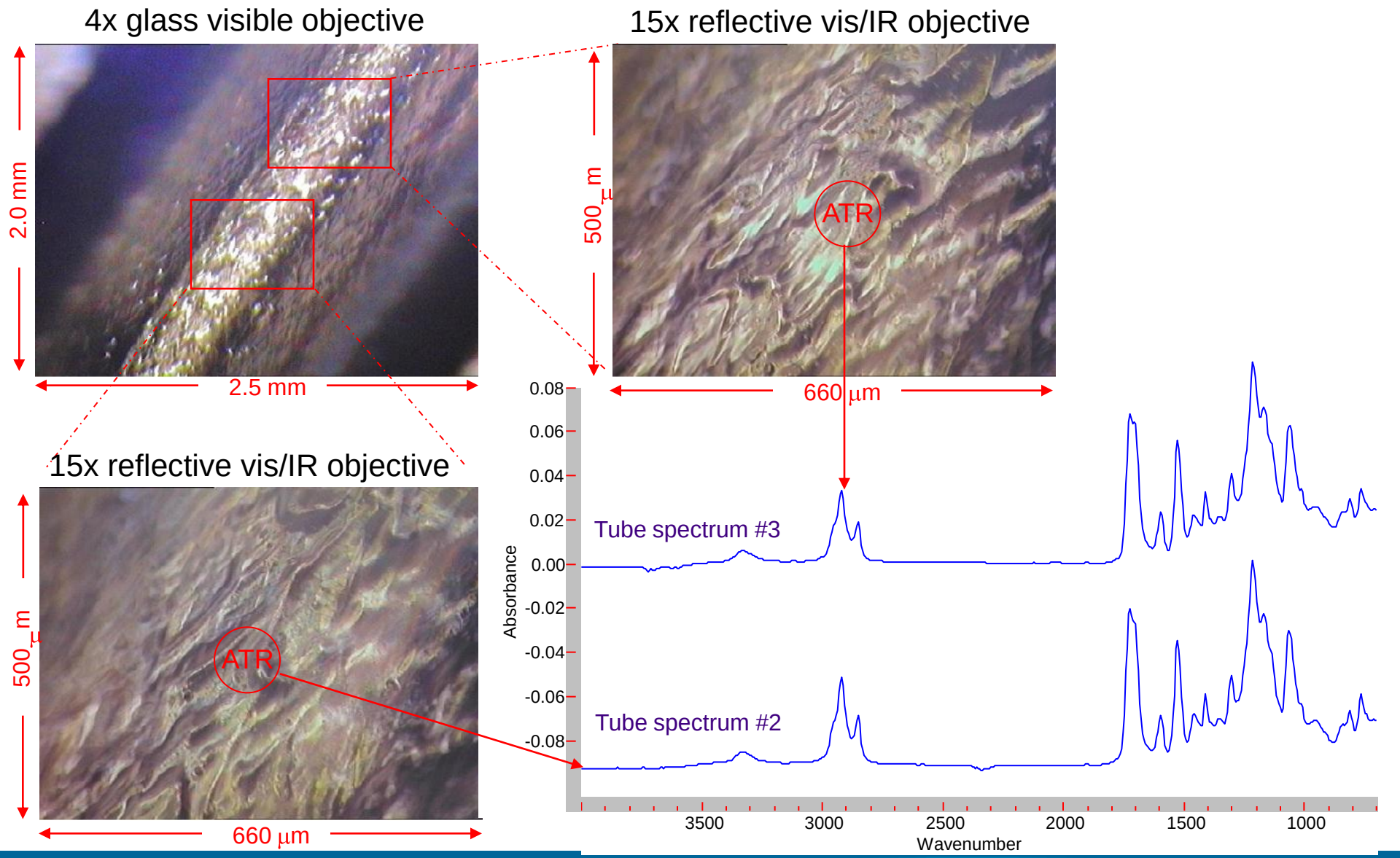




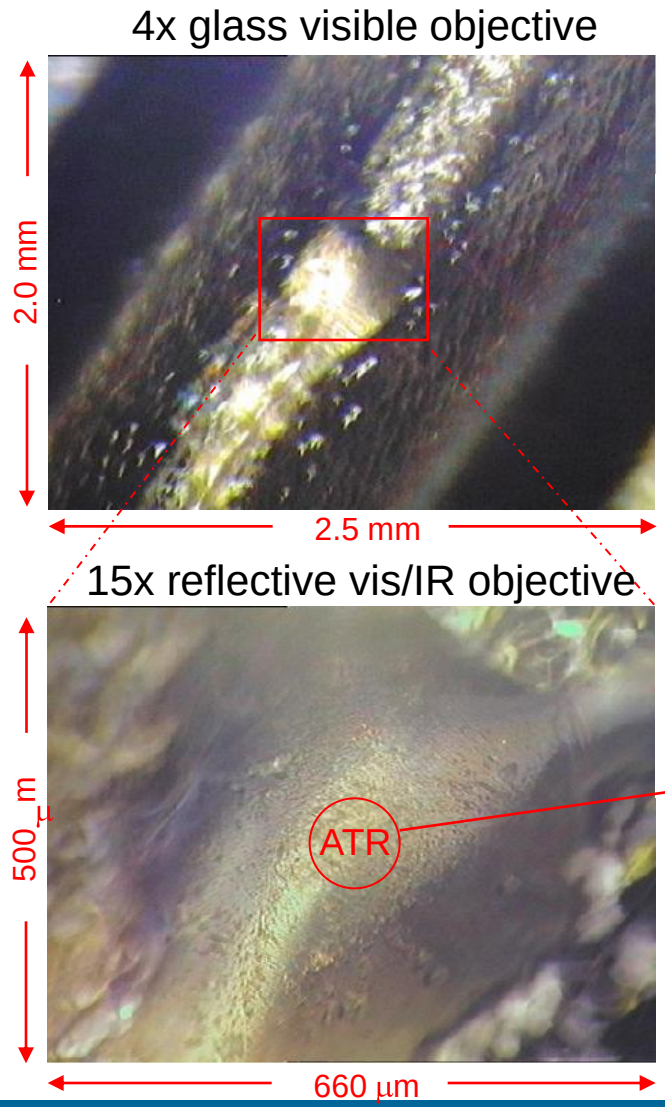


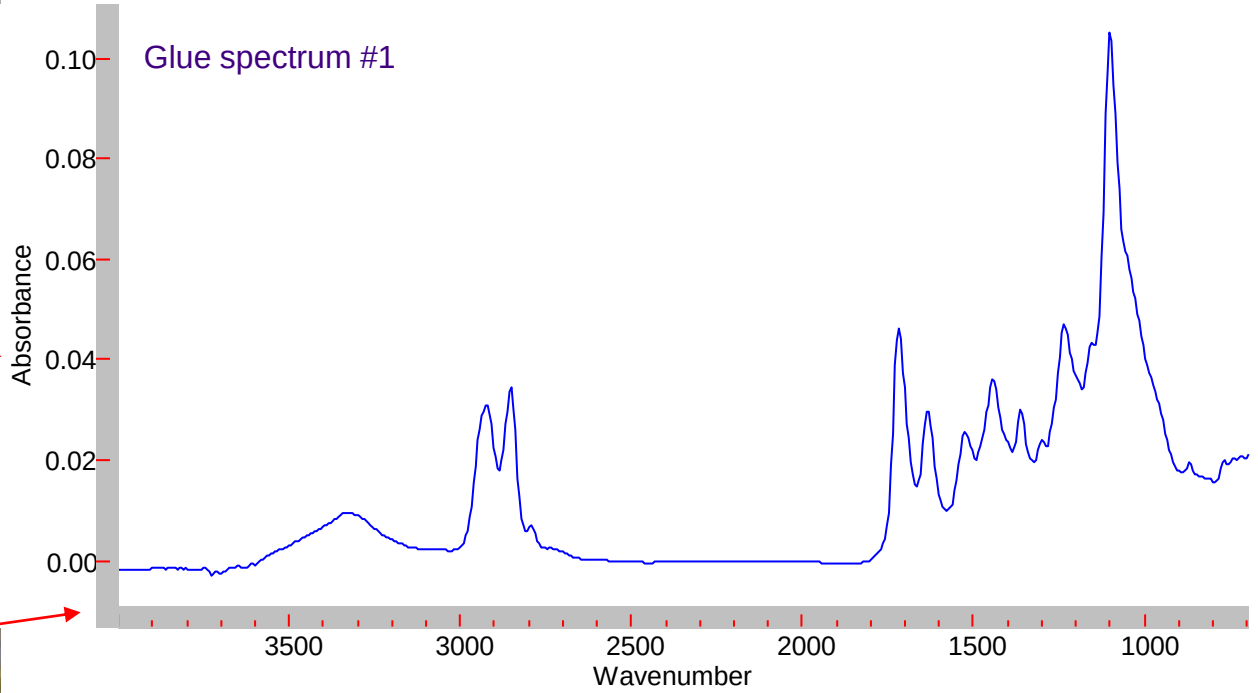


Results - Tube spectrum #2 & #3



Results - Glue spectrum #1





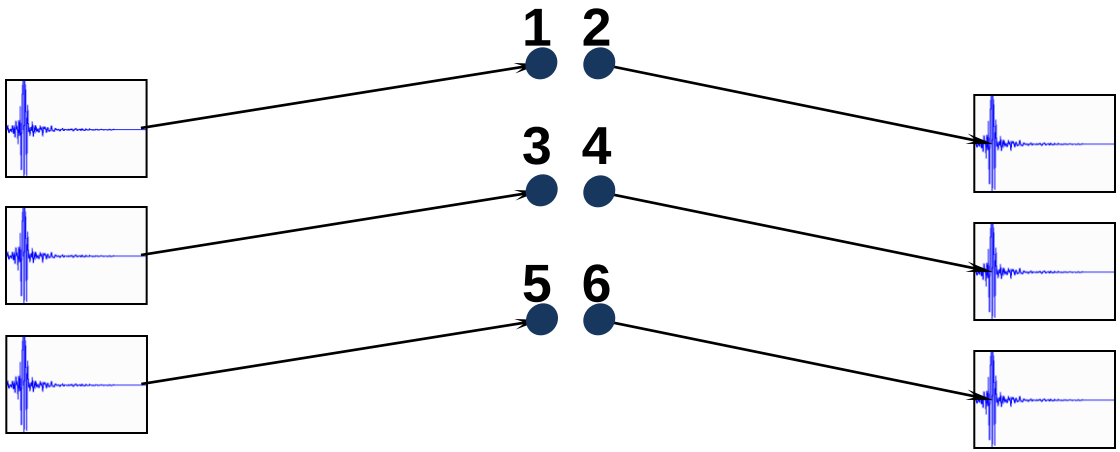
Infrared Mapping

- ***Single Point***

- ***Linear Arrays***

Infrared Single Point Mapping

- One data collect at each point gives one interferogram or spectrum
- Move the sample with a motorized stage and collect multiple scans
- Build up a Map of the sample



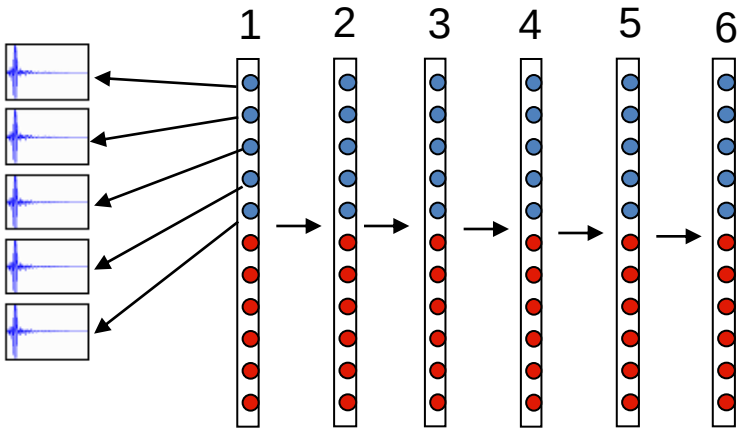
Automatic Single Point Mapping

The automated mapping experiment can be used to obtain IR spectra over a sample.

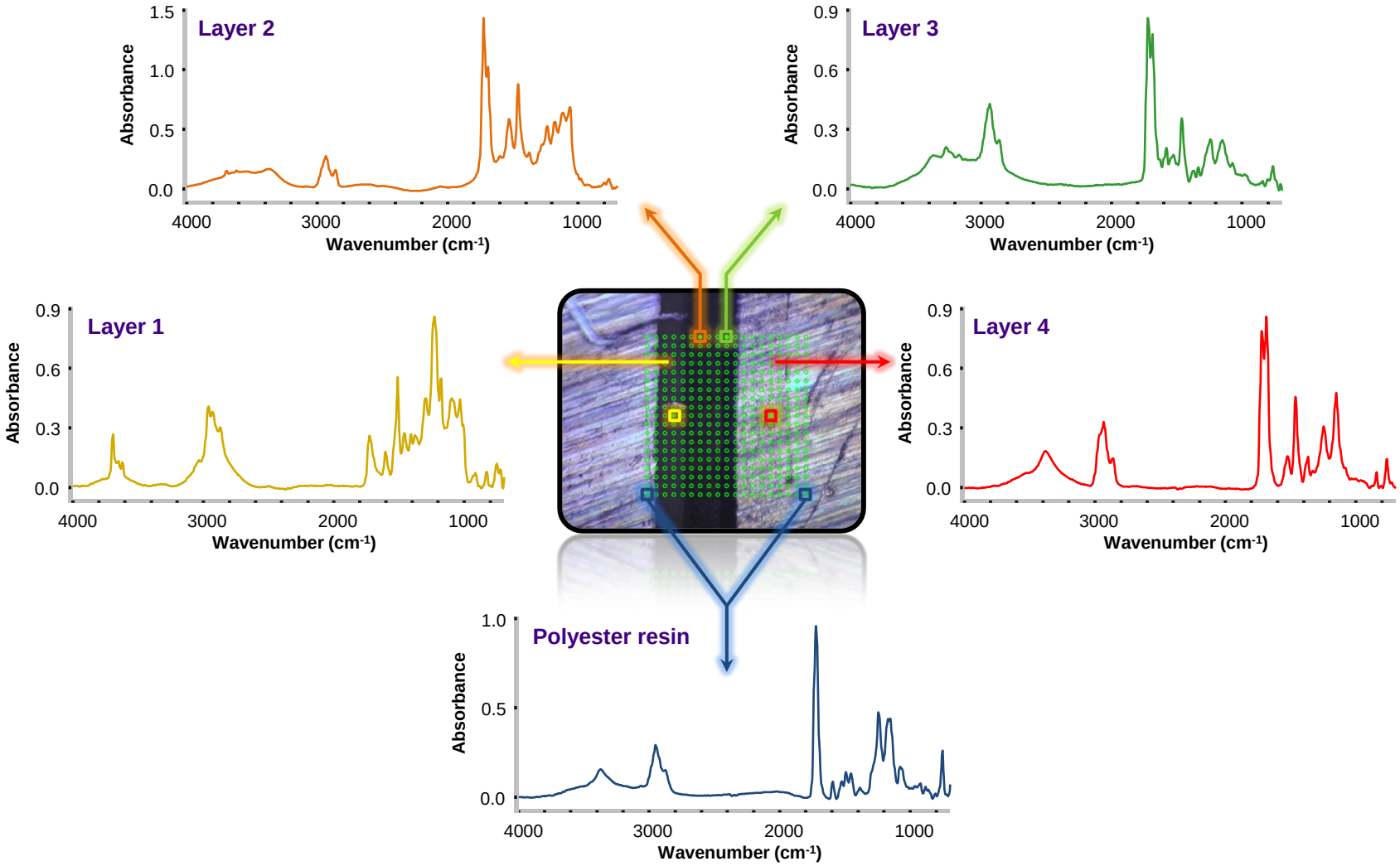
- Define the field to be mapped.
- Define spacing of the points to be collected (x and y direction).
- Define aperture/spatial resolution (the area you are collecting data on an individual scan).
- You must have visual control of the experiment.
  You are visually locating areas of interest.

Infrared Linear Array Mapping

- A row of data from each pixel in the array (usually 1 x 16 or 2 x 14) collected simultaneously
- Move the sample with a motorized stage and collect multiple scans
- Build up a Map of the sample by “stitching” linear array scan together
- Faster than single point mapping, but still much slower than FPA imaging



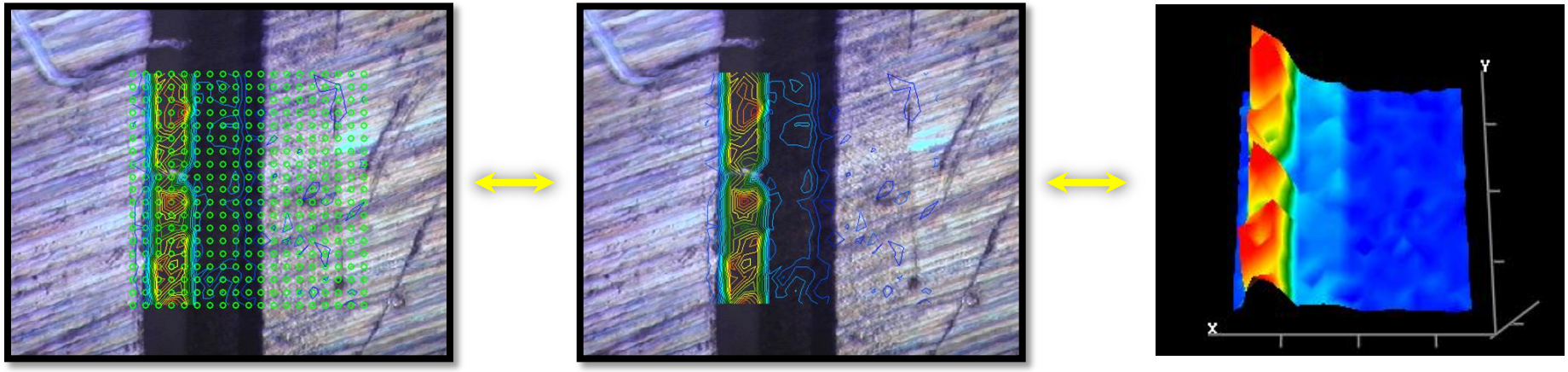
Infrared Mapping in Material Analysis: Multi-layer Paint Sample



Infrared Mapping in Material Analysis: Multi-layer Paint Sample

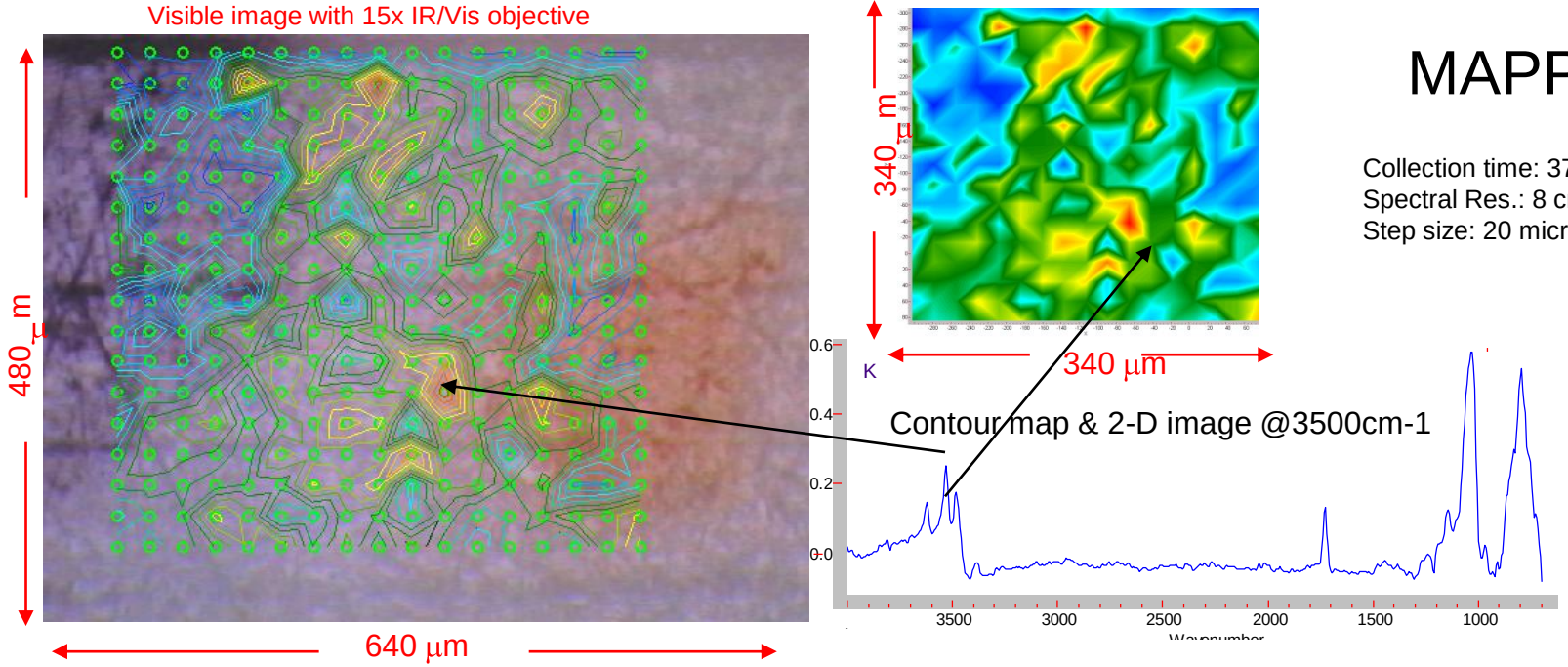
Feature image based on absorbance at 3692 cm^{-1}.

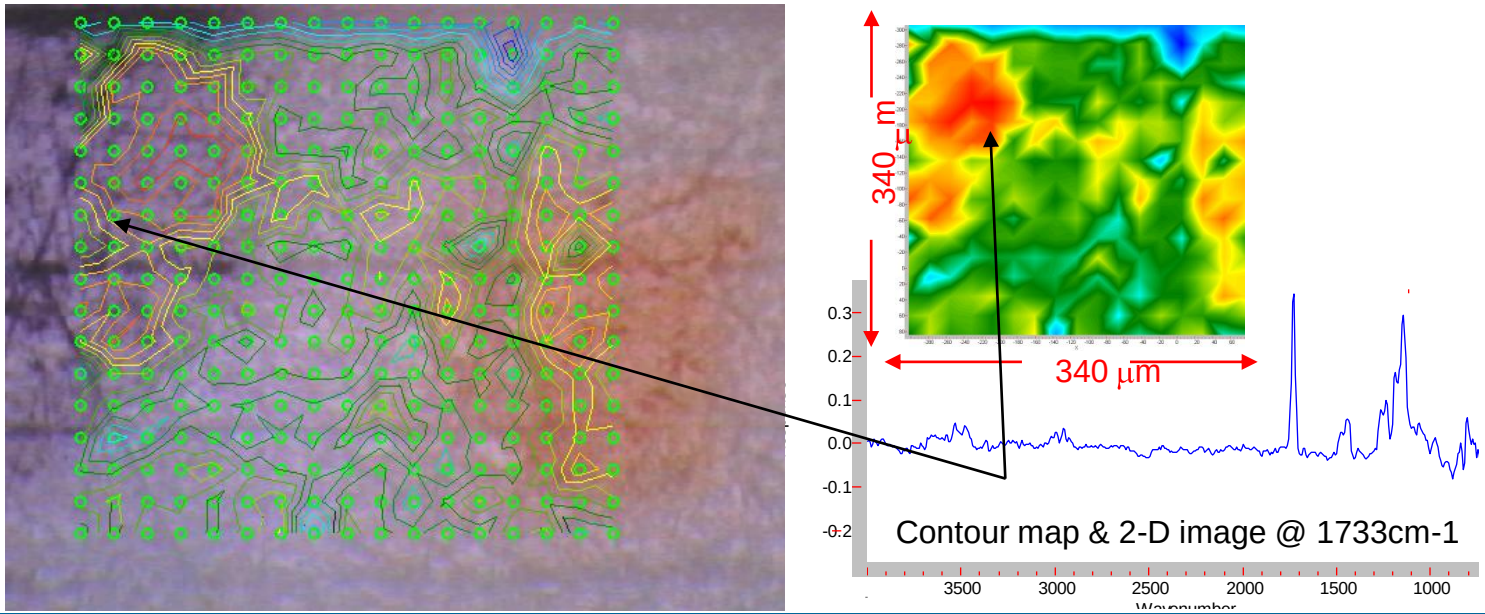
Abs. at 3692 cm^{-1}



MAPPING

Collection time: 37min
Spectral Res.: 8 cm-1
Step size: 20 micron



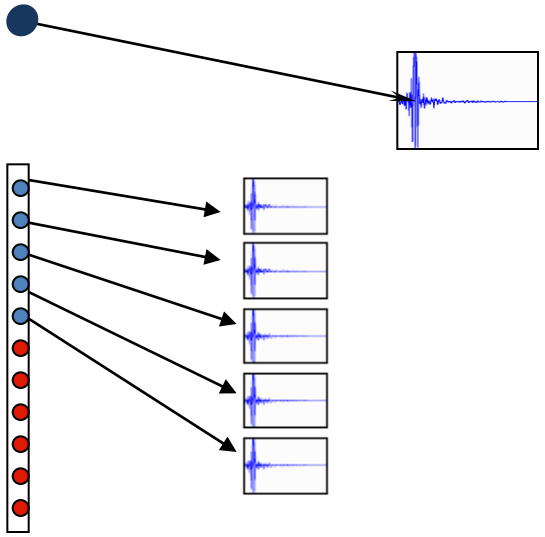


Infrared 2-D Focal Plane Array Imaging

Progression of techniques….

Single point Mapping

- 1 spectrum/scan
- Move sample to create map

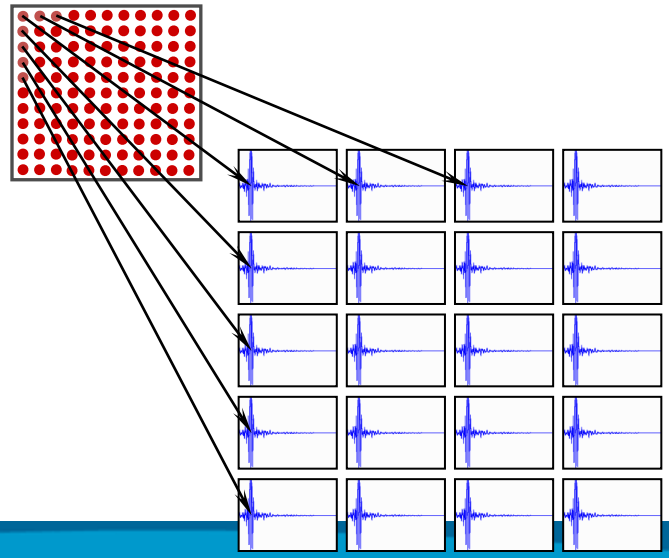


Linear Array Mapping

- 16 spectra/line scan
- Move sample to create map

2-D Focal Plane Array (FPA) Imaging

- Image collected as a single “snap shot”
- 1 sec for 4096 spectra (64x64 pixel FPA)



→ Faster data collection

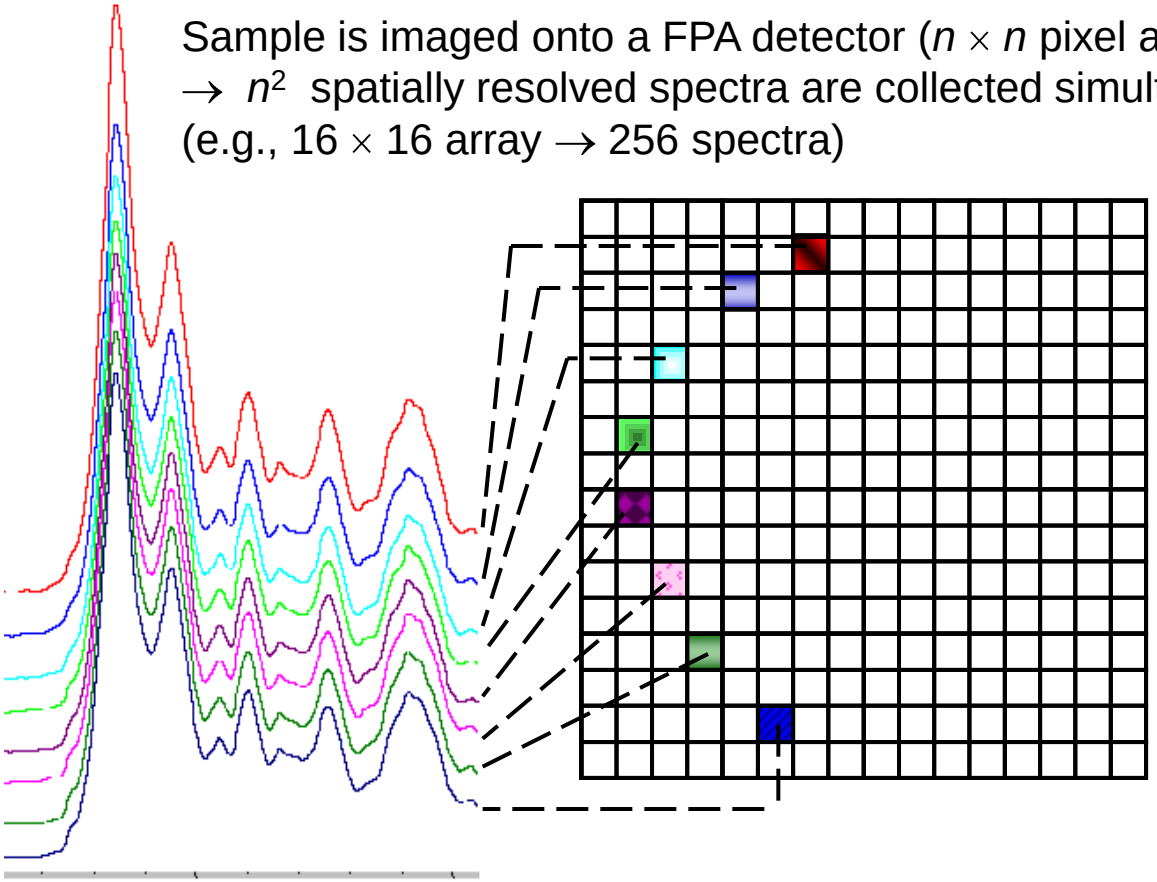
→ Better interfacial information

→ Higher spatial resolution

Principle of Infrared Imaging

FPA-FTIR detectors provide the ability to acquire a grid of spectra in the same amount of time that it takes single point detectors to acquire one spectrum

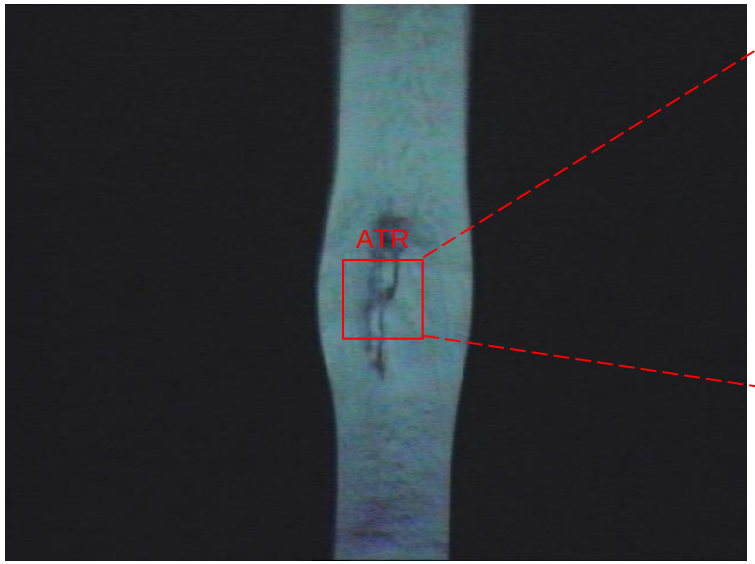
Sample is imaged onto a FPA detector ($n \times n$ pixel array)
$\rightarrow$ n^2 spatially resolved spectra are collected simultaneously
(e.g., 16 $\times$ 16 array $\rightarrow$ 256 spectra)



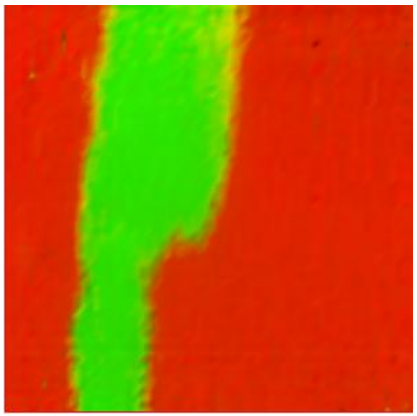
One pixel (~5.5µm)
is an entire spectrum

Sample D – Cross-sectioned across defect

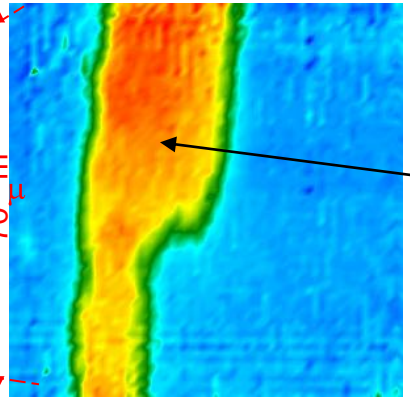
Visible image with 15x objective

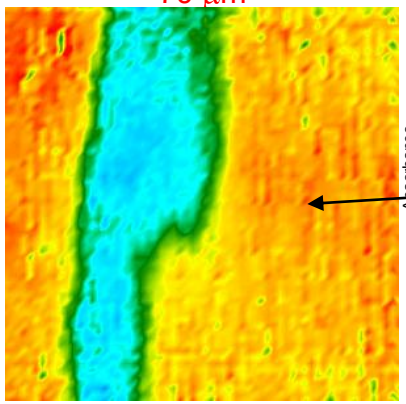


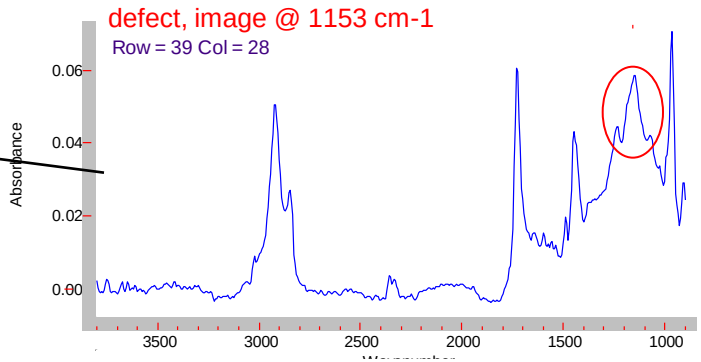
Composite (Green/Red) image

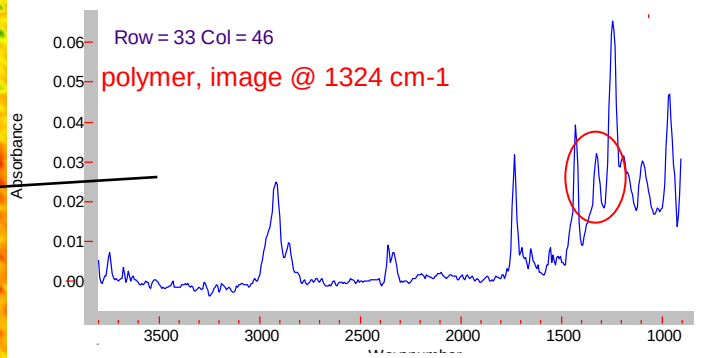


GREEN – DEFECT
RED - POLYMER

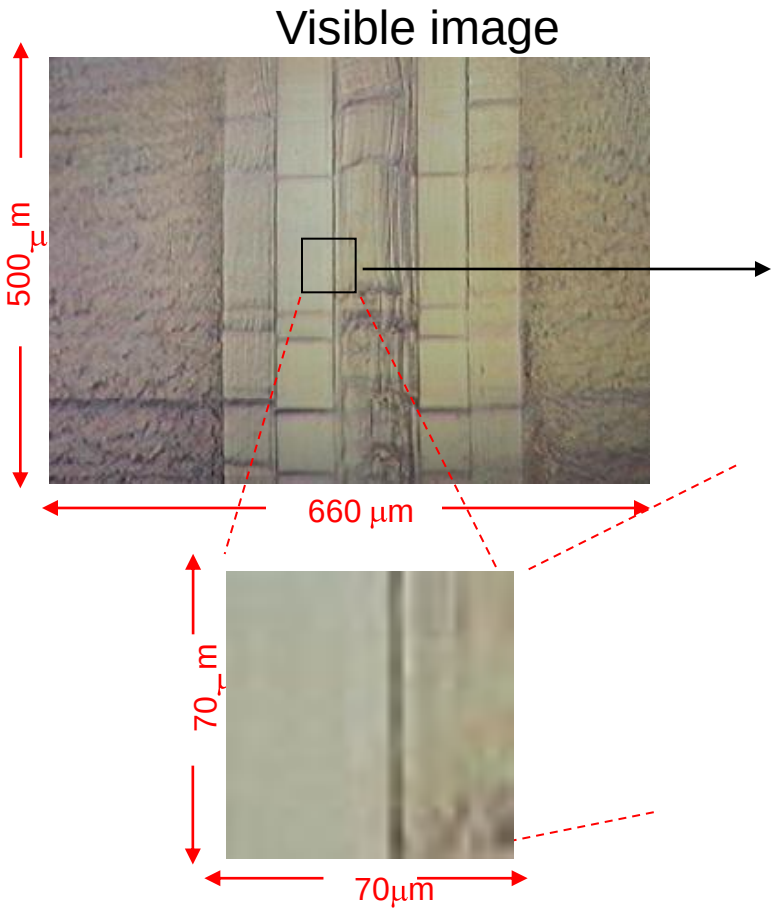


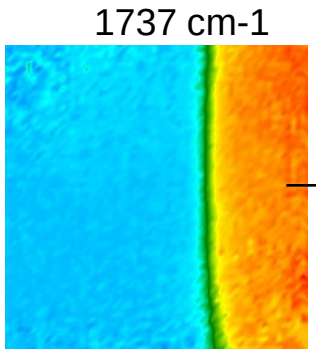


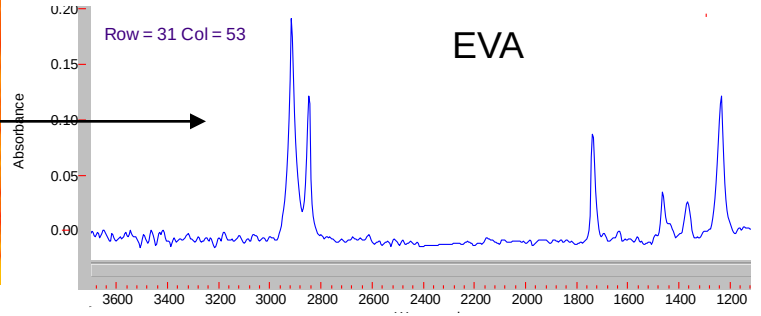


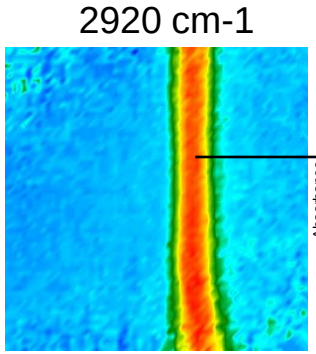


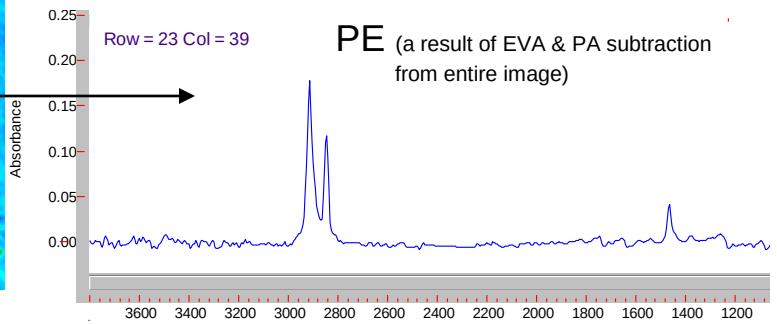
9 layer laminate: cut “in-house” medium layer – initial exploratory analysis

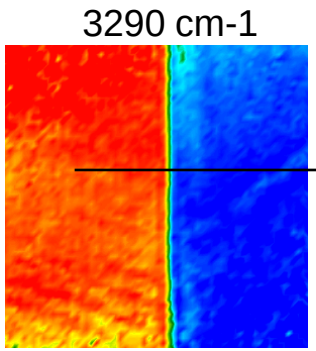


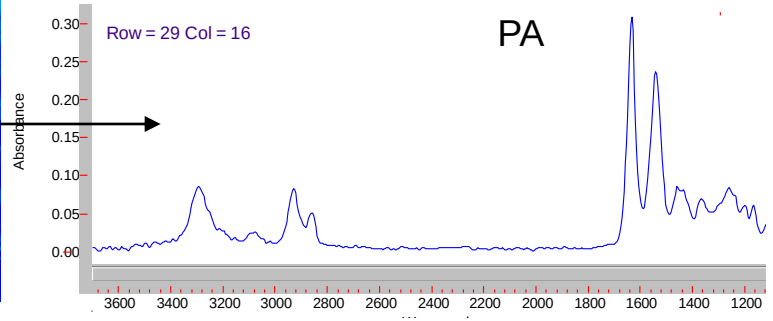












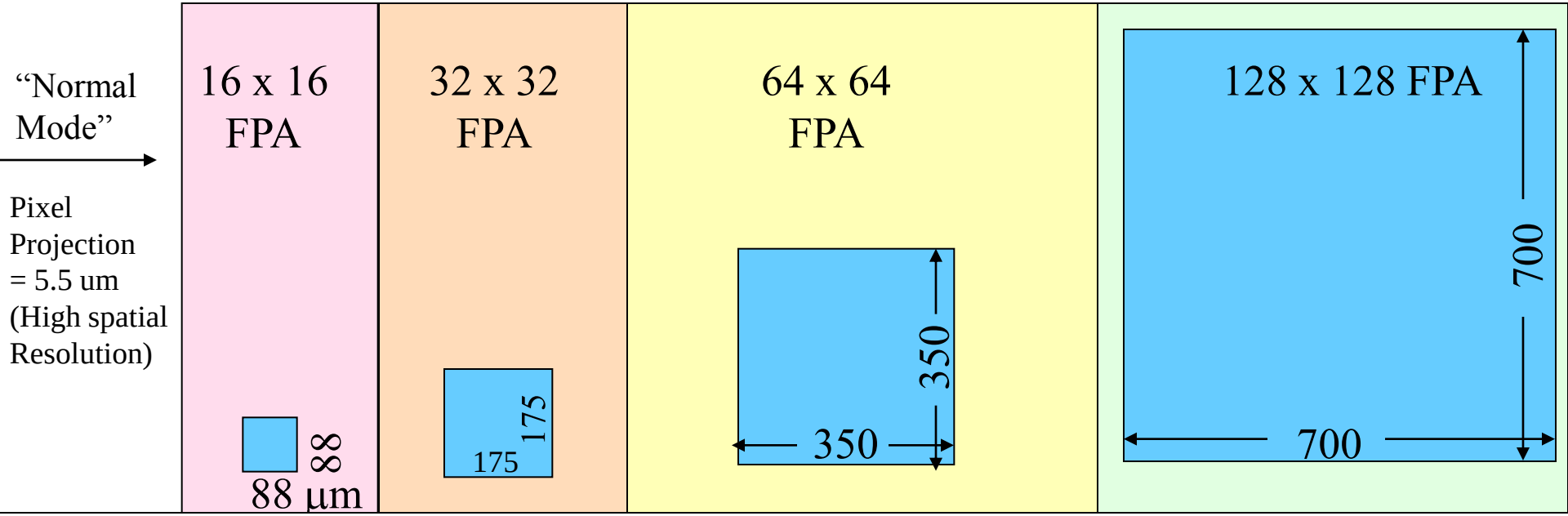
Enabling Technology

Infrared FPA detectors bring an entirely new capability to the field of IR analysis.

The technique provides the ability to simultaneously measure spatial (**WHERE**) and spectral (**WHAT**) information.

- Provides the ability to spatially locate sample inhomogeneities
- The data is collected in parallel and differentiates this technique from mapping in single point or linear array mode
- Agilent's modern FPA technology, enable data to be collected in "rapid scan" mode

Agilent's FPA's - Wide choice to match needs



The Agilent 620-IR microscope

-designed for FPA imaging

Agilent 610-IR Microscope (Single element)
Silver Bullets

- Best Performance - Better SNR and energy throughput than ANY other microscope system on the market
- Flexibility with ease-of-use
  - Reflection / Transmission / ATR analysis (Multiple objectives)
  - Binoculars as standard
  - Simplified control panel
  - Options for high resolution visible cameras

Upgradeability to Dual Single element & Infrared Imaging

Agilent 620-IR Microscope (Imaging)
Silver Bullets

In *ADDITION* to the features and benefits of the Agilent 610, the Agilent 620 includes:

- Superior sensitivity, speed and analytical performance

  Better SNR and energy throughput than ANY other microscope system on the market

  Highest resolution. FPA provides for significant speed advantages over

- Largest Field of View (FOV) for chemical imaging

  True chemical imaging with a 2-D Focal Plane Array (FPA)

  Field Expanding Optics (FEO)

- Flexibility with simplicity (ease-of-use)

- Superior data visualization tools & analysis software

Top 4 Features, Values, Benefits
Microscope

No.	Feature	Value	Benefit
-	2-D FPA	Increased S/N, spatial resolution and speed	More higher quality information faster
-	Field Expanding Optics	Quadruples the area of analysis for imaging collects	Increased efficiency and speed
-	Infinity Corrected Design	Allows use of standard Olympus high magnification objectives and other optical components	Provides for greater experimental flexibility
-	Unique “LIVE” ATR imaging	Allows for immediate and ultra sensitive feedback on the point and quality of ATR contact	More sensitive measurements with little or no impact on sample

MARKETS AND APPLICATIONS:

A. Chemical Analysis

B. Life Sciences

Part III A

Chemical Analysis

Agilent Technologies provides comprehensive solutions in chemical analysis industries

Industries include:

Environmental
Food & Flavors
Forensics
Hydrocarbon Processing
Polymers & Materials
Semiconductor
Specialty Chemical
Homeland Security

Environmental

Agilent offers over 40 years of environmental analysis and regulatory expertise.

Contaminants

- Pharmaceuticals and Personal Care Products
- Endocrine Disruptor Compounds
- Perluorinated organic compounds
- Dyes and Pigments

Water

- Volatiles
- Semi-volatiles
- Pesticides and Residues
- Inorganics

Soil & Sediment

- Volatiles
- Semi-volatiles
- Pesticides and Residues
- Inorganics

Air

Material Analysis (Heavy Metals)

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Air

Material Analysis (Heavy Metals)

FT-IR can be used for the identification of emerging contaminants however, the detection limits are part per thousand typically a few % – so not useful for trace levels compared to chromatography but applicable to bulk.

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Emerging Contaminants
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- Endocrine Disruptor Compounds
- Perluorinated organic compounds
- Dyes and Pigments

Water
- Volatiles
- Semi-volatiles
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- Inorganics

Water has a strong absorption in FT-IR that limits its use.

However, there are several notable applications, including:
- the detection of oils in water
- forensic analysis of an oil or biodiesel spill (with GC/MS)
- marine microbiology (blue-green algae) & nutrient studies
- high conc. water treatment chemicals

Soil & Sediment
- Volatiles
- Semi-volatiles
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Air

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Soil & Sediment

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- Inorganics

Air

Material Analysis (Heavy Metals)

- EPA method 8440 – Total recoverable petroleum hydrocarbons by FT-IR
- DIN 38 409 H18
- EPA method 8410 - GC/FT-IR for semivolatile organics
- Volcanology – trapped gas in rocks
- Land management (landfill remediation applications) and environmental geochemistry
- Mineral composition
- Adsorption/desorption during mineral processing (time effects – kinetics)

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Emerging Contaminants
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- Endocrine Disruptor Compounds
- Perluorinated organic compounds
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- Volatiles
- Semi-volatiles
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- Inorganics

Soil & Sediment
- Volatiles
- Semi-volatiles
- Pesticides and Residues
- Inorganics

Air

Material Analysis (Heavy Metals)

Dedicated accessories for gas analysis allow for the measurement of vapor species to ppb levels.

Applications include:
- Landfill gas analysis,
- Isotopic ratio studies ex: HCl/DCl
- Monitoring levels of atmospheric gas, concentration of CO_2 or sulphur-containing compounds
-- Nuclear fuel related gas measurements (purity determinations of UF6 gas)

Food & Flavors

Infrared spectroscopy is an important analysis method for the world's food, animal feed, pet food, and nutrition industries.

Used for the identification and quantification of:

- Food and beverages
- Flavours
- Food packaging
- Foodbourne pathogens
- Edible oil testing
- Food contaminants & adulterants
- Fermentation control
- Vitamins
- Food additives
- Nutritional food supplement products

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- Food additives
- Nutritional food supplement products

Temperature controlled transmission accessories and various ATR accessories can be used to analyze liquids, aqueous solutions and food ingredients for QA/QC purposes.

Applications include:

- Analysis of whole grain, flour, meat, milk, and cheese

- Alcohol, sugar and water content in beverages (wine, spirits, juice)

- Composition of Milk (protein, fat, lactose, total solids)

- Degree of meat spoilage using ATR

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- Foodborne pathogens
- Edible oil testing
- Food contaminants & adulterants
- Fermentation control
- Vitamins
- Food additives
- Nutritional food supplement products

FT-IR is particularly useful for the analysis of modified atmospheric packaging (MAP – used to prolong shelf life), Biodegradable, and Edible food packaging.

Applications include:

- Study of active antimicrobial films in food packaging (thermal stability and mechanical properties)

- Study of specific migration of heat stabilizers from rigid PVC into food (investigate migration phenomena and diffusion coefficients)

Food & Flavors

Infrared spectroscopy is an important analysis method for the world's food, animal feed, pet food, and nutrition industries.

Used for the identification and quantification of:

- Food and beverages
- Flavors
- Food packaging
- Foodborne pathogens
- Edible oil testing
- Food contaminants & adulterants
- Fermentation control
- Vitamins
- Food additives
- Nutritional food supplement products

FT-IR is routinely applied to edible oil analysis.

1. QC/QA analytical:
   - Type of unsaturation
   - Trans fat content (AOAC method)
   - Iodine value
   - Saponification number
   - Peroxide value
   - Solid fat index
   - Anisidine value (frying applications)
   - Free fatty acids
2. Classification/discrimination (adulteration) – Halal applications
3. Emulsions (imaging applications) – Beverage & food processing apps.

Forensics

FT-IR spectroscopy is a widely used technique in Forensic Sciences.

It provides fast, accurate and reliable sample analysis.

Sample analysis is typically non-destructive.

Infrared microscopy can be used for small samples (less than 1 – 2 mm down to a few microns).

Dedicated spectral libraries can help to identify the analyzed materials.

Forensics

Common applications include:

- Hair and fiber analysis
- Ink on paper analysis (counterfeit money & forgeries)
- Paint chips recovered from vehicles
- Tablet analysis (illicit drugs and counterfeit)
- Trace analysis left by fingerprints
- Unknown white powders
- Residues on metal surfaces
- QA/QC of mixtures of amphetamines, barbiturates, GHB, etc.

Hydrocarbon Processing
(Oils and fuels)

Dedicated Oil Analyzer

- Lubricant and hydraulic fluid condition monitoring (degradation and contamination).

Monitoring applications include:

- Petroleum-based lubrication oils in diesel, gasoline and natural gas engines, including buses, railroad, fleet vehicles, and construction equipment
- Synthetic ester-based lubrication oils in jet engines and power turbines
- Predictive maintenance and condition monitoring
- Petroleum and synthetic-based hydrolic fluids
- Gearbox oils and transmission fluids
- Fluid quality control

Hydrocarbon Processing
(Oils and fuels)

Biodiesel (FAME) analysis:

- FT-IR affords a simple approach to the quantitative determination of fatty acid methyl ester in diesel blends.

- ASTM D7371 and EN 14078

Specialty Chemical

FT-IR spectroscopy is an ideal tool for QA/QC of raw materials and finished products.

- Easily analyse solids, liquids, gels, and gases on a single FT-IR platform
- Routine identification and verification analysis
- Detection and identification of low concentrations of organic and inorganic samples (synthesis products and reaction intermediates)
- Easy-to-use analyzer software to simplify routine analyses

Specialty Chemical

Customers:

- Raw chemical manufacturers & chemical processing plants
- Petrochem refineries & natural gas companies (ex: Exxon, Shell)
- Mining companies (ex: Schlumberger)
- Government labs (esp. military, environmental protection agencies, toxicology agencies, risk assessment groups)
- University/college professors and lab managers

MARKETS AND APPLICATIONS:

A. Chemical Analysis

B. Life Sciences

Part III B

Life Sciences

Agilent Technologies provides comprehensive solutions in life science industries

Industries include:

Genomics
Metabolomics
Proteomics
Biopharma
Drug Discovery
Drug Development
Disease Discovery
Drug Manufacturing QA/QC
Traditional Chinese Medicine

MOLECULAR PRODUCT PORTFOLIO

UV product line overview

Cary 50

8453

Cary 100/300

Cary 4000/5000/6000i

Fluorescence product line overview

Cary Eclipse

Cary Eclipse MPR

Molecular product line overview

HIGH END	MID RANGE	ENTRY LEVEL
Cary 4000 Cary 5000/6000i 670/680-IR 610-IR scope 620-IR imaging	8453 Cary 100/300 Cary Eclipse 660-IR	Cary 50 640-IR*

* 640-IR fits with “upper end” Entry Level

QUESTIONS