COMPARISON OF
Miniaturised Near Infrared Spectral Sensing Technologies

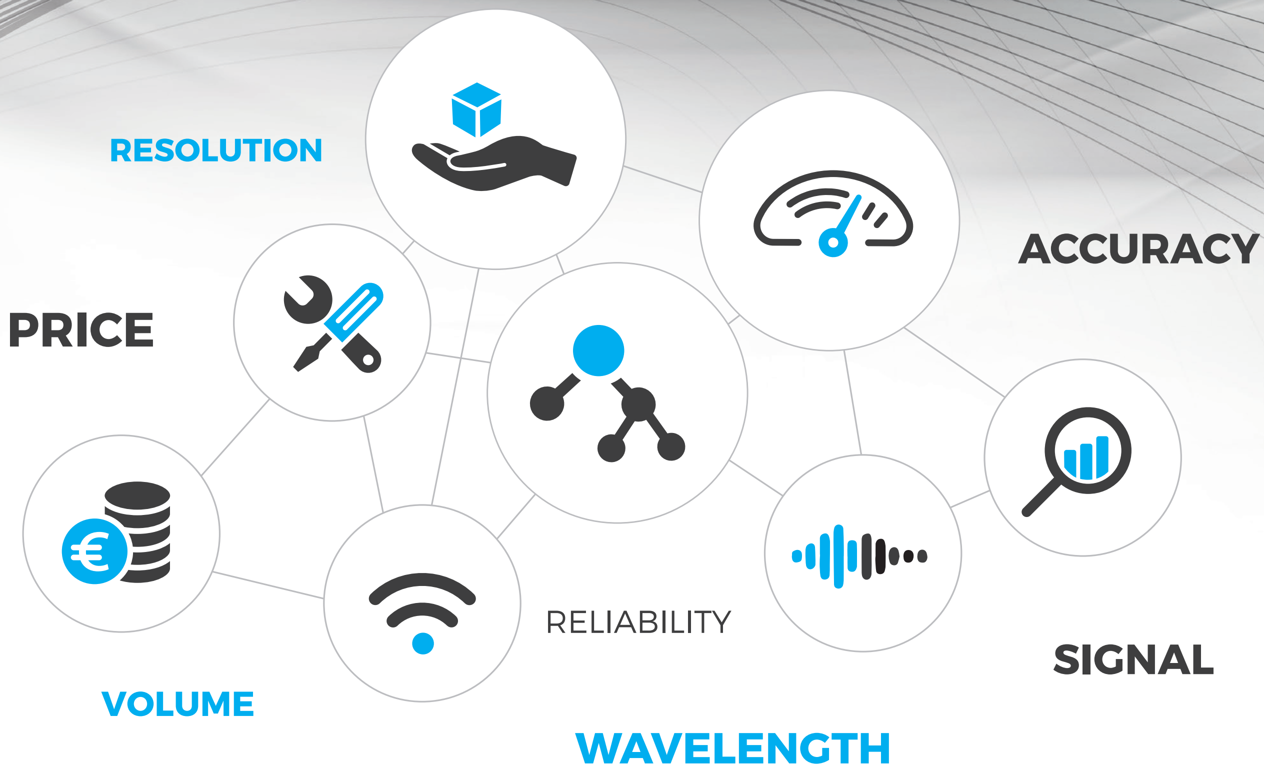


Table of content

Introduction

The field of spectroscopy is moving fast from the 80's laboratory work through 90's in-line and 2000's portable devices to real mobile and widespread applications during 2010's. In this development, there are many technical and application-related challenges of which the most dominant is the cost and the size of the hardware. To overcome this, many trials have been made to develop the next-generation spectroscopic devices, which would at the end become spectral sensors rather than spectrometers: small and low-cost devices that are seamlessly connected, providing meaningful information to the user.

The most prominent wavelength range concerning the information content, availability of detectors and light sources, and ease of sample preparation is the Near Infrared (NIR) wavelength range. Generally this range is concidered including wavelengths from 750 to 2500 nm. To this region various new techniques have been developed to meet the future demand, most of them concentrating in the development of Microelectromechanical (MEMS) manufacturing technologies.

This whitepaper will summarize the current status of the main technologies and solutions around miniaturized NIR spectrometers on their way to become true spectral sensors. The whitepaper gives practical guidelines on how to choose a technology for an application.

The field of spectroscopy is changing rapidly. In this whitepaper we will summarize the current status of the main technologies and solutions and give practical guidelines on how to choose a technology for an application.

NIR technology and market development

Near Infrared (NIR) spectroscopy is a field of analysing and identifying material and material content by illuminating an object with infrared light, gathering transmitted or reflected light by the spectrometer, and using various mathematical data analysis methods to deliver results. The first very extensive commercial applications of NIR were developed in the agriculture and food industries, one example being the project led by Canadian Grain Commission to use NIR technology as a basis for buying and selling wheat based on analyses of protein, oil and moisture. Analytical applications of NIR spectroscopy developed rapidly in the 1980´s, thanks to progress in key enabling technologies: the personal computer, optoelectronic technology and multivariate modelling or chemometrics (statistical and mathematical methods applied to the field of chemistry).

Today analytical measurements are the most significant application area for NIR spectrometers in laboratory studies, process monitoring as well as hand-held and field measurements. There are thousands of application papers published so far of NIR spectroscopy for varying analytical measurements in agriculture and food industries, forestry, environmental, medicine, pharmaceutical, chemical, textile, cosmetics and many other applications.

The advantages of NIR analysis are often mentioned as:

1. minimum sample preparation
2. rapid analysis
3. no reagents needed
4. non-invasive and non-destructive
5. simultaneous multi-component analysis possible
6. sample size from very small to very large, depending on the equipment
7. compatible with fiber optics, in which case the sample may be separated from the instrument

The types of spectrometers used are:

- Fourier Infrared Spectrometers (FTS, FTIR or FT-NIR)
- Grating (dispersive) spectrometers (monochromators and compact multipixel spectrometers)
- Fabry-Pérot Interferometer spectrometers (FPI)
- Fixed filter arrays and filter wheels

The first very extensive commercial applications of NIR were developed in the agriculture and food industries. Today analytical measurements are the most significant application area for NIR spectrometers in laboratory studies, process monitoring as well as hand-held and field measurements.

The benchtop FTIR has many benefits, like high throughput, wide wavelength range and good resolution and it is therefore the most used high-end NIR analyser, manufactured by companies such as Bruker. Grating spectrometers have become compact in the recent years, especially in the so called Very Near Infra Red (VNIR) range. Compact NIR grating spectrometers are today the most common devices when going to process control applications due to smaller size, higher robustness and lower cost than the FTIR. The drawback of using compact grating spectrometers is that in the sensitive wavelength ranges, the multi-pixel detector technology needed is expensive and often produces modest signal-to-noise ratio (SNR).

Lately this obstacle has been tried to overcome by Texas Instruments by providing their micromirror (DMD) technology to replace the multi-pixel detector with a scanning mirror and a single pixel detector. Also the FTIR is being miniaturize by companies such as Si-Ware. As the computation power and connectivity has been significantly improved over the years via digitalization of societies, new possibilities for expanding the possibilities for NIR spectroscopy have risen. Therefore, another type of spectrometer, earlier used mainly in astronomy and telecommunications, has been introduced to markets in the recent years, being the first that can really catch the high-quality, meaningful applications of the true NIR wavelength range, while being capable of scaling up in volumes to hundreds of thousands or millions, while dropping the price tag to sub-100€ level. This technology is called the Fabry-Pérot interferometer.

Tematys, a market research company based in France, envisions in their recent marketing report from December 2016 that the market for miniaturized spectrometers will be doubled in the next 5 years, and the trend in the 2010's is going to point-of-care and consumer applications. Previously, the problem preventing this significant growth (the NIR market has been growing only at a few % CAGR in the recent years) has been the size and cost of the instrumentation, but now new approaches have emerged to overcome this.

According to a recent report from Tematys, the market for miniaturized spectrometers will be doubled in the next 5 years. Pictured here are NIRONE Sensors from Spectral Engines, based on the Fabry-Pérot interferometer.

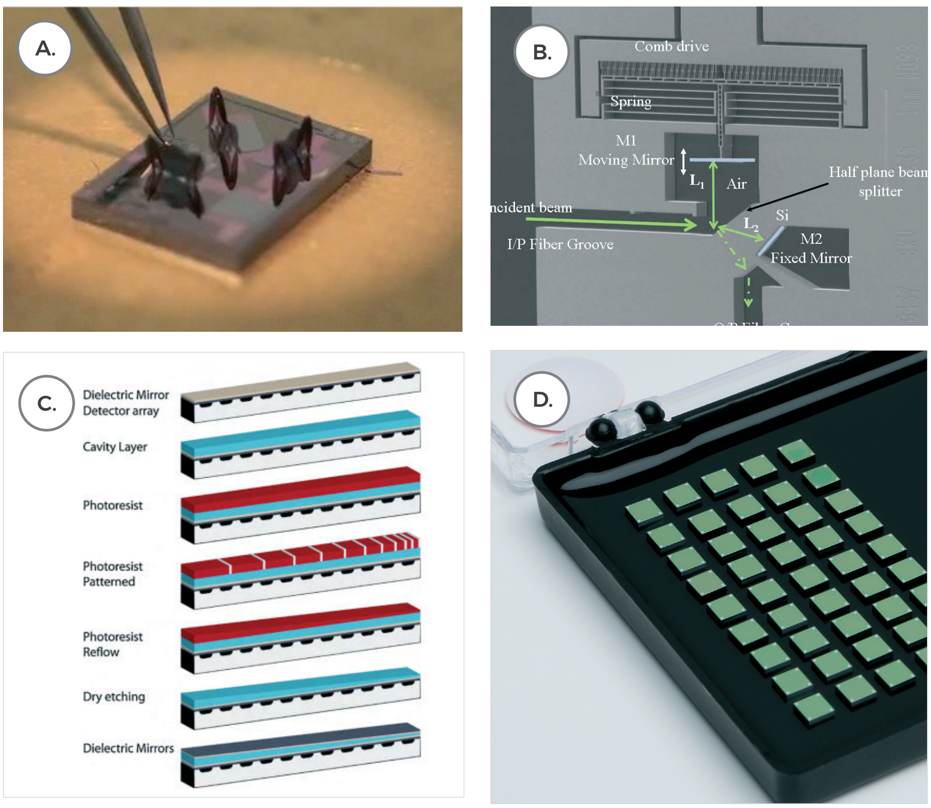
Miniaturization principles and challenges

There are many limitations concerning miniaturization, most relating to manufacturing techniques. Taking separate, macroscopic parts, and trying to make them smaller only gets one so far. Limitations of manufacturing techniques of mechanics and optical parts come into play, destroying tolerances, but leaving assembly and calibration costs high. In order to reach the next level, new philosophies are needed.

Currently the dominant manufacturing technology used for miniaturising spectrometers is MEMS, or Microelectromechanical systems. This enables much smaller features and more integrated structures than was previously possible. MEMS technologies employ deposition, patterning and etching techniques, taking place in a clean room, to form mechanical and electrical structures in a microscale. Eventually one can get hundreds of chips from a single silicon wafer, resulting in highly scalable and low-cost devices. The main philosophy is to take a traditional spectrometer type, such as Fourier Transform Infrared (FTIR), Fabry-Pérot (FPI) or grating-based spectrometer, retain the working principle, but scale down the size with this new manufacturing technique.

Micromechanical sensor devices and techniques have become widespread after the A-class Mercedes failure in the 'moose test' in 1997. Accelerometers were quickly needed to produce active stabilization to the car, as it was too easy to flip over with a quick steering motion. Since then, MEMS sensors of various kinds have become a commodity in cars, and later in mobile phones. A mass production example of optical MEMS is the DLP projector technology by Texas Instruments.

Figure shows examples of MEMS solutions for making spectrometers:



Examples of different kind of MEMS-based spectrometer structures. A) In-plane FTIR with flip-up components (Block Eng.), (Copyright 2009, SPIE) B) in-plane integrated FTIR (Si-Ware), (Copyright 2009, IEEE) C) Static FPI (Linear Variable Filter) (Delft), (Copyright 2010, Elsevier) D) off-plane monolithic FPI's (Spectral Engines).

Other common methods of breaking the barrier of common mechanics manufacturing tolerance limitations are nanoimprinting and LIGA. Both of these methods are used to manufacture and replicate very fine grating structures, and also to create monolithic optical benches for grating spectrometers.

One philosophy in the miniaturization and lowering the cost of instrumentation is to limit oneself to working below 1000 nm in the wavelengths (the 'VNIR' range), as this is a cut-off for the very inexpensive silicon detector technology. Here the price of a multi-pixel sensor is not an issue and LED light sources are also readily available. Lately, companies like Consumer Physics and AMS have demonstrated this route. The selection of this wavelength range presents a major obstacle: the molecules do not react well and all the spectral fingerprints start to get mixed, because one is actually measuring the 3rd or 4th overtones of molecular vibrations. The sensitivity and the specificity (how well can you distinguish materials from each other) can be anywhere between 10 and 1000 times worse in the VNIR than in the 'true NIR' range from 1000-2500 nm. This is compensated by setting up large databases and performing analysis in the cloud, using machine learning and other sophisticated methods, but one can only get to a very indicative level, even with the smartest of algorithms.

For some applications where one needs, for example, to measure through a thick sample, the VNIR range is applicable, but the vast majority of applications lie in the true NIR range. Figure below illustrates this: to get to meaningful mass applications, one needs to get from the top part to the lower boxes. To start creating a digital ecosystem with some indicative first applications, one can function in the lower left box. But to eventually create meaningful, sustainable applications, one must reach the green box on the lower right side. The vast majority of the examples of miniaturization presented in this paper are concerning specifically this green box – this is where Spectral Engines is one of the leading companies.

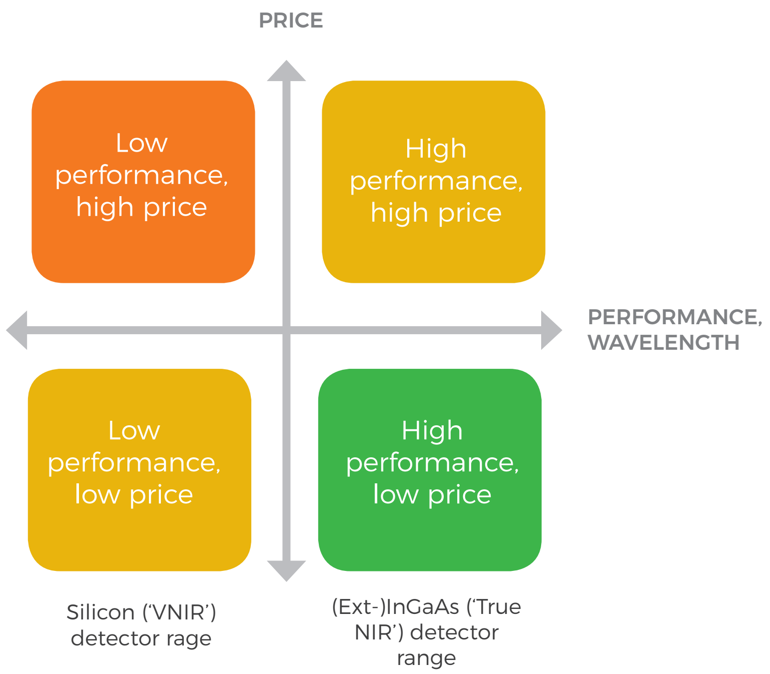


Illustration of instrument division per performance and price.

In the case of realizing a spectrometer using MEMS technologies, one usually concentrates in producing a mirror movement of some sort to create an active interferometer. At the same time, however, one should keep the optical area large to sustain usable signal-to-noise ratio of the system. Movement can be achieved in multiple ways, like using piezoelectric, electrostatic or thermal actuation. Piezoelectric and thermal actuation are very susceptible to hysteresis and ambient temperature changes, and therefore they always need an additional measurement circuitry to repeatedly control the motion. Because of this, the vast majority uses electrostatic actuation, as it draws almost no power, and it can be stable enough to avoid external stabilization circuitry. This makes the overall system simpler, easier to calibrate and therefore cheaper. The general benefit of silicon-based MEMS compared to macroscopic solutions – in addition to the small size and cost – is that even though there is motion, there is virtually no wear and one easily achieves billions of repetitions without a notable effect.

Many have been only concentrating on the MEMS chip itself, creating only the single moving mirror, but we should not forget that this is only one part of the entire system: you also need a light source, focusing optics, band-limiting filters and a detector, along with the electronics. And, you need to attach the MEMS somewhere without destroying or distorting it, package it hermetically while keeping the optical path available and maybe align some multimode fibers with it. In spectroscopy, the movement usually needs to be rather large, while the controlling needs to be very accurate and repeatable, as errors in the wavelength axis of even 0.5 nm might destroy an application. Also, one practical parameter to consider is the mass that is moving: as the mirror size often needs to be large, the mass of the moving part is often rather high compared to spring forces holding the mass, which makes the system susceptible to vibrations and to directional offsets due to gravity - imagine a weight hanging on a spring.

So, it doesn’t help if one manages to make a large MEMS mirror, moving hundreds of micrometers, but finding it impossible to control without an external reference laser, the movement being very slow, needing a cooled detector and a shoebox worth of sophisticated electronics and optics. If the MEMS component costs a few euros to manufacture, but the end result is a badly performing box at 20 000€, the business case does not really match. In other words, it is very important to design the MEMS and the whole system integration so that the entirety becomes small, easy to assemble and robust, otherwise the end-result will not be usable in large scale.

Concentrating on the MEMS chip itself and creating only the single moving mirror is only one part of the entire system. It is very important to design the MEMS and the whole system integration so that the entirety becomes small, easy to assemble and robust, otherwise the end-result will not be usable in large scale.

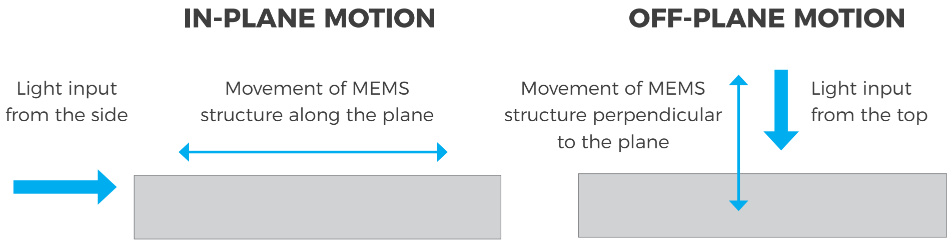
Current main types of realizations and main actors

The commercial miniaturization of NIR spectrometers has started from making traditional grating spectrometers as small as possible, and by introducing a new type of compact spectrometer in the 2000's by JDSU (MicroNIR), where they utilized special thin film technology to create a linear variable filter, a type of Fabry-Pérot interferometer (FPI). Also, the first commercial MEMS solution came out with Axsun's NIR engines. Simultaneously, lots of work on developing new MEMS solutions were on their way at VTT (Finland), Fraunhofer (Germany), Si-Ware (Egypt), University of Western Australia (Australia) and Hamamatsu (Japan), to name a few. Coming out to the 2010's, these solutions began their commercial try-outs one-by-one with Hiperscan, Si-Ware, Hamamatsu, Texas Instruments, TellSpec and Spectral Engines. People are already looking towards consumer applications, and more work to further decrease the price and size of the spectrometers are continuously happening.

Consumer Physics (Israel) for example, targets consumer markets directly with successful crowd funding campaigns and the first mobile phone integration concept. There are naturally trade-offs when going small and cheap: signal-to-noise levels suffer, device-to-device calibrations become more challenging, selecting low-cost silicon as detector material means low detection of materials etc. If the performance is too low, then meaningful, sustainable applications will not carry the business - the same thing happens if the price is too high. All the companies and technologies are balancing between these topics, and often the right answer depends on the application.

Table below summarizes current miniaturization technologies and related spectrometer solutions by type. The table also sums up the current main actors and general pros and cons of the solutions. We have categorized the technologies first based on their spectral functioning principle, and then by how the optical axis of the system is organized concerning the movement of the MEMS mirror/plate. In MEMS, one always has a chip, which is rather thin (0.5 mm) and the top area is rather large (5-50mm^2). 'In-plane' means that the light is coming into the system from the small 'side' of the chip, resulting in a small optical area, but easier to organize large movements, whereas 'off-plane' motion means that the light is coming in perpendicular to the surface. There the optical throughput can be high but large movement more difficult to organize. The third category is 'fixed', meaning that there are no moving parts at all and the spectral separation is organized spatially: a multi-pixel detector is necessary.

Table below explains these two main types. We also categorize the tilting mirror being within the off-plane motion.



The two main types of MEMS chips based on the direction of optics and mechanical motion.

One way to categorize these different technologies would be "scanning" or "spatial", but this is in fact represented in the detector type category, as all the scanning systems use a single pixel detector and spatial systems a multi-pixel detector. Spatial systems are usually faster and require no active motion control, but the cost of multi-pixel detectors in the true NIR is too high to be taken to masses: the detector element price can be several hundreds of euros when moving away from silicon-based detector technologies. The silicon-based detectors limit the usable wavelength range to below 1000 nm, this being a serious drawback of the low-cost detectors, because there is very limited amount of molecular information below 1000 nm (the so called 3rd and 4th overtones of the actual molecular vibration modes).

The price of NIR pixelated detectors is not the only drawback of related solutions: they experience higher noise levels and usually need to be cooled (added complexity and cost) and they experience a noise source called pixel-to-pixel variation, which naturally is non-existent in the case of a single pixel system. In addition, depending on the geometry of the sample and the optical setup, different pixels might 'look at' different physical location on the sample, producing errors in the interpretation of spectra in the case of heterogenous samples. Finally, multi-pixel solutions are usually too large to be really miniaturized. As a general benefit, the multi-pixel detectors are often the right choice with fast moving targets. Because of the price level, size and performance challenges of the multi-pixel systems, the main commercial effort in the recent years have been concentrating on scanning systems and using NIR single pixel detectors (InGaAs and extended InGaAs).

Main technology category	Motion category	Description of the system principle	Detector type	Main Actor(s)	Main Pros	Main Cons
FTIR	In-plane	Integrated interferometer with plate comb drive	Single pixel	Si-Ware, Hamamatsu	Wide wavelenght range, whole optical bench integrated	Low optical throughput, susceptible to shocks and vibrations
	In-plane	Discrete moving mirror component in macroscopic optical bench	Single pixel	Thermo Fisher	Wide wavelength range	System price due to complex assembly and large chip
FPI	Off-plane	Surface micromachined FPI, stacked with detector in a hermetic metal can	Single pixel	Spectral Engines, Hamamatsu	Very compact, high mass-producibility, robust, fast, high throughput	Limited wavelength range for single component
	Off-plane	Several high-order FPIs	Single pixel	Axsun	High throughput, wide range, high resolution	Very complex system, high cost, large
	No motion	Linear variable filter on a linear array detector	Multipixel	Viavi	Compact, robust, no motion	Expensive, size-limited
Grating	Off-plane	Scanning grating	Single pixel	Hiperscan	Wide wavelength range, stable wavelengths	System price due to complex assembly and large chip, low throughput
	Off-plane	Scanning micromirror + discrete grating	Single pixel	Texas Instruments, TellSpec	Programmable wavelength selection, wide spectral range, fast	Complex optical bench, size and cost-limited
	No motion	Integrated grating	Multipixel	Insion, Zeiss	Integrated optical bench, robust	High price, size-limited
	No motion	Discrete grating	Multipixel	Horiba, Ocean Optics, Avantes, Hamamatsu	Robust, well-known	Expensive, size-restricted, high SNR needs cooling
Multichannel	No motion	Multiple small band-pass filters on a multipixel detector	Multipixel	Hamamatsu, AMS, Consumer Physics	Compact, low-cost if silicon, no actuation	Expensive if InGaAs, low sensitivity if Silicon.

Summary table of commercial types of MEMS-based NIR spectrometers.

One obvious thing to note on the different actors is that their business model varies. Companies like Hamamatsu sell quite low-level components, leaving the instrument realization and calibrations to the customer, whereas for example Thermo Fisher sells an entire portable analyser, which just happens to include their MEMS component. So, when comparing technology, one should also look at the effort needed to create a new system, because there is a huge amount of effort put and know-how created in many of these companies on how the MEMS can be made to reliable work in actual application conditions.

One interesting topic in the various technologies is their future potential. What are the limits, are they at their limit? Especially if one is selecting a new platform, it is good to understand how this platform might look like in 5 years. The MEMS FPI technology, for instance, shows highest miniaturization potential because of its small chip size (<3x3x0.5 mm3) and extremely simple optical system layout (stacked on top of a single pixel detector).

More details on the various MEMS approaches can be found in MEMS- and MOEMS-Based Near-Infrared Spectrometers. Encyclopedia of Analytical Chemistry (Antila, J., Tuohiniemi, M., Rissanen, A., Kantojärvi, U., Lahti, M., Viherkanto, K., Kaarre, M. and Malinen, J. 2014, 1–36). There are also trials to make spatial, or non-moving, FTIR devices using multi-pixel detectors, development on tunable NIR laser sources and other special approaches. Also, there are additional approaches and actors when going past the NIR wavelengths to Mid Infrared (MIR), but these are not covered in this whitepaper.

Comparing basic specifications

As the principles for the spectral measurements differ, the technical specifications cannot always be directly compared. This is especially tricky, if a person has been accustomed to using one type of technology, and then tries to transfer those specifications to a new type of device. There are two major practical differences to look at: the total measurement time & signal-to-noise ratio, and instrument function.

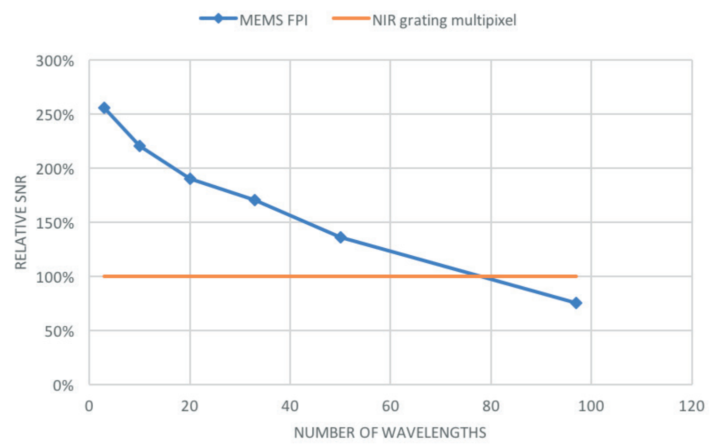
The total measurement time and signal-to-noise ratio

The time you spend on getting your measurement result is usually the real specification you want, and not, for example, integration time, which is actually only one of the parameters contributing to the total measurement time and the signal-to-noise ratio (SNR). Selecting the time, one can tune several parameters in the spectrometers to achieve as good an SNR within that time as possible. The main difference is that scanning devices need time for the mechanical scanning when spatial devices don't.

A special ability exists in the scanning FPI's and micro-mirror -based grating spectrometers: as one can select the position and amount of wavelengths by software, one can also optimize the wavelength points for an application. Figure below shows a practical example of this when Spectral Engines FPI-based sensor has been compared with a grating spectrometer at 1940 nm, using the same total measurement time of 200 ms, same fiber coupling, target and light source, and changing the amount of spectral points to be measured.

As the amount of spectral points in a grating spectrometer is fixed, there is no change in the signal level, but as the amount of points are decreased for the FPI, one can compensate this by added averaging and thus get a better SNR. In many practical applications, like moisture measurement, 10 points is well adequate, so SNR improvements of 2-5 are easily achievable with this optimization.

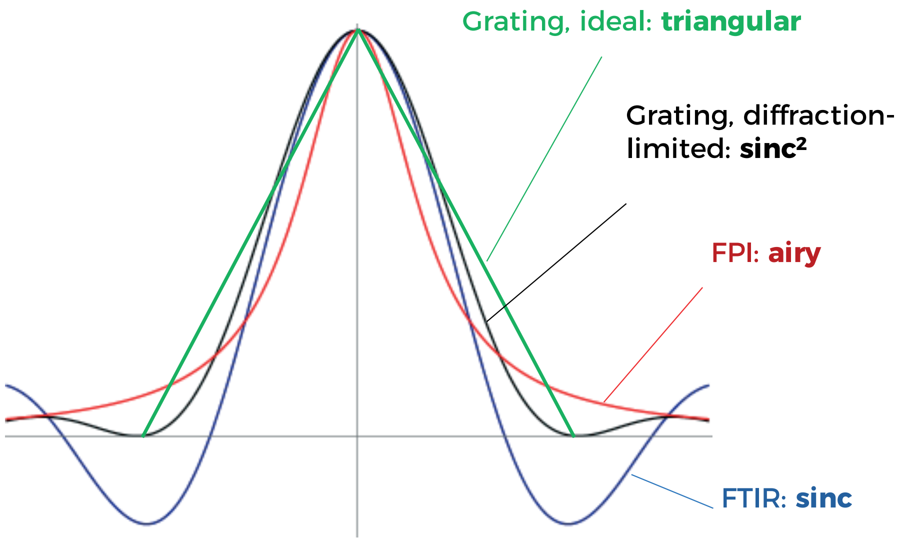
Total time therefore consists of scanning time, integration time, number of averaging and data readout, transfer and analysis but which of these parameters are relevant or governing depends on the spectrometer type.



Comparing a grating spectrometer with a cooled detector and a Spectral Engines FPI device. Total measurement time for both was 200 ms and the amount of wavelength points to be measured with the Spectral Engines' device was changed.

Instrument function

All the different types of spectrometers (FTIR, FPI, Grating and Multichannel) have a different response to the spectrum. A NIR spectrometer never exactly replicates the real spectrum, but ads its own instrument shape to the results. This is called convolution. This makes it difficult to translate a database built with one type of device, to be used by another type. When people are talking about the “resolution” of their device, this can therefore mean different things. The wavelength resolution for most devices are depicted by the Full Width at Half Maximum (FWHM) value, but even this is not directly comparable as the ‘sideslobes’ around the main peak are of different shape, and different portion of the main energy fall within the FWHM, typically from 70% to more than 90%. The FTIR has a different definition all together: the resolution of an FTIR device is the width of the first zero crossings on both side of the main peak. And, to make it even more complex, that value can be affected by a different kind of pre-processing called apodization. Figure below illustrates the difference between technology types.



Various instrument functions for different spectrometer types.

Table on the next page summarizes most of the spectrometer specifications for different types of devices. The values in the table can be held as indicative, as e.g. there are many companies manufacturing grating spectrometers and thus the size, weight and many other things can vary significantly. One quickly sees that for some technologies the manufacturers do not for some reason give specifications, and some specifications are not relevant to some of the technologies. One also needs to pay attention on the definition of specifications, as terms like accuracy, repeatability and the resolution might mean different things.

Specification comparison table with notes for common types of spectrometers. Table has been compiled by using data gathered from public sources in 2017. Spectral Engines does not take responsibility of the accuracy of this table but recommends always to check from the manufacturer.

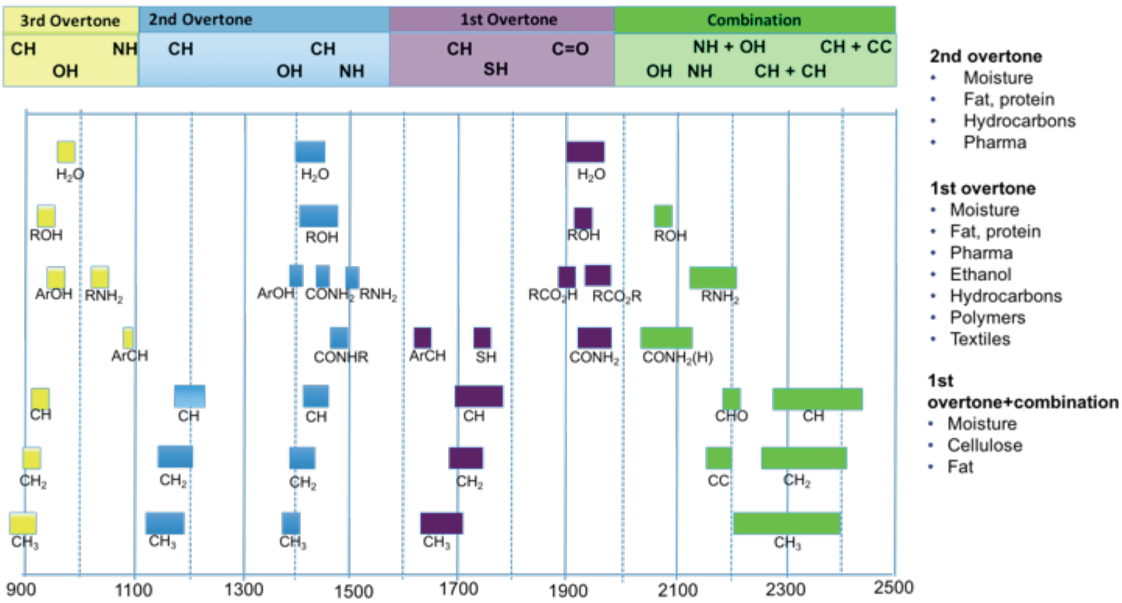
	Things to consider	Surface-micromachined MEMS FPI	MEMS FTIR	LVF	General grating	Monolithic grating	Grating with TI DLP	Multichannel detector
Wavelength ranges	These depend on technology and detector type used	1.3 - 1.7 µm 1.5 - 2.0 µm 1.7 - 2.2 µm 1.9-2.5 um	1.25-1.7 um 1.3-2.1 um 1.35-2.5 um	0.95-1.65 1.15-2.15	0.9-1.7 um 1.1-2.2 um 1.1-2.5 um	0.9-1.7 um 1.1-2.2 um	0.9-1.7 um	0.6-0.9 um 0.75-1.0 um
Detector	Single pixel detector area is 100x bigger and cost 100x less than that of the multipixel detector.	Single-point (Extended) InGaAs	Single-point (Extended) InGaAs	(Ext-)InGaAs array	(Ext-)InGaAs linear array (with 2 stage TE-cooling), 256 or 512 pixels	(Ext-)InGaAs array, 128 or 256 elements	Single-point InGaAs	Silicon multipixel sensor
Spectral separating element	The basic technology type for separating the spectrum	MEMS Fabry-Perot	MEMS FTIR	LVF	Grating	Monolithic grating	MEMS DMD from Texas instruments	Fixed filter array on Silicon array detector
Optical interface	Many devices have been only fiber-coupled	Open or fiber	Open or fiber	Open or Fiber	Fiber	Fiber	Open or fiber	Open
Entrance slit	Relevant for grating spectrometers	Not relevant	Not relevant	Not relevant	10-200um	60µm x 300µm	60µm x 300µm	Not relevant
Resolution	Commonly FWHM figures.	Typical <13..20 nm	8 nm or 16nm @ 1550 nm, FWHM	Typical 10..20 nm	4-90 nm (depends on grating and slit)	10..16 nm	10..12 nm	20 nm
Wavelength repeatibility	Measurement-to-measurement or device-to-device?	+/- 0.3 nm (device-to-device)	+/- 0.1 nm	< 1 nm	+/- 0.3 nm	Not given	Not given	Not given
Temperature induced drift	Very rarely given by companies. Optical benches with discrete components experience hysteresis.	< 0.03 nm/°C	Not given	Not given	0.05-0.1 nm/°C	<0.05 nm/°C (from VIS version)	Not given	Not given
Mechanical scanning time	Scanning modes can be different: stepwise or continuous.	1 ms between wavelengths	Not given	Not relevant	Not relevant	Not relevant	15 ns	Not relevant
Wavelength step size	Different between scanning (programmable) and fixed pixel devices	0.01 .. 400 nm	Not given	6 nm	2..10 nm	4..8 nm	Not given, programmable	Not given
Signal-to-noise ratio	Often announced for some measurement time or amount of averaging at ideal lighting conditions.	>10'000 @ 0.5s	>3'000 @ 2s	23'000 with 100 averaging	5'000	5'000	5'000 typical	Not given
Integration time	Integration time is fixed for single pixel devices. Signal quality there is increased only by averaging.	30 us per wavelength	2.5 ms min	10 us min	10 us - 1000 ms, depends on type	2 - 40.000ms	Not given	Not given
Operating temperature range	Very limited if active cooling is applied. MEMS range can often be tailored.	+10..+50°C	-5..+40°C	-20 to 50°C, non-condensating	+5-50 C (+5-35 C), non-condensating	5°C below ambient .. 40°C (cooled)	0..50°C	+5-50C, non condensating
Power requirement	Questions: Lamps included, cooling included, idle condition or 'full speed'?	<0.3W	<2.5 W	<2.5 W	<2.5 W, <40W (with detector cooling)	7.5W (cooled)	Not given	<0.02W
Size	Envelope size. Some measures include light sources, some include bluetooth etc. extra boards.	ca. 25x25x20 mm, including light sources	80x65x45 mm	45 (diam) x 48 (height) mm, including light sources	300 x 200 x 100 mm	108 x 76,6 x 21,5mm	82.2mm (L) x 66mm (W) x 45mm (H)	4.5 x 4.7 x 2.5
Weight	Check what is included	< 15 g	150 g	60 g	1-3 kg	130g	136 g	Not given
Shock	Usually not given. If given, refers to certain standard, but not the same from tech to tech	IEC 60068-2-31	Not given	Drop test ISTA 2A	Not given	Not given	Not given	Not given
Vibration	Usually not given. If given, refers to certain standard, but not the same from tech to tech	MIL-STD-810G	Not given	MIL-PRF-28800F Class 2	Not given	Not given	Not given	Not given

Practical comparisons

In the end, how can you tell how a specification affects the final result? If possible, the first thing one should do is to make a measurement series using e.g. a high-end bench-top FT-NIR with high resolution and wide wavelength range. From that data, you can pin down the actually needed wavelength ranges mathematically.

In NIR spectroscopy one finally measures molecular vibrations: different materials react to light at different wavelengths depending on their molecular bonds. The same molecules react at different 'overtone' ranges, that is e.g. water can be measured at multiple wavelengths. Therefore, if you need a moisture sensor, you don't need but a certain range in the spectrum. **The higher the wavelengths, the more sensitive and specific one gets and the lower, the more insensitive and ambiguous the spectral shapes get.** In the specifications table on the previous page, the FPI platform looks like it has a major restriction. Despite this, because of the wavelength range of a single device, the vast majority of NIR applications can be covered with this technology, as one very rarely needs to cover multiple overtone regions in a high-volume, commercial sensing application.

Figure below illustrates the overtones and molecular bonds to be detected.



The NIR absorption bands and typical application areas.

Even after going through all specifications, it is still down to testing the application at hand to see how the devices perform. What does a narrower spectral range do to your final error, is it better to have a good SNR or good resolution? VTT Technical Research Centre of Finland made practical comparison measurements between three different types of spectrometers in three applications: 1) polyethylene coating thickness on paper, 2) paper moisture content, and 3) paracetamol, lactose and microcrystalline cellulose in pharmaceutical blends. To overcome the ambiguity of specifications, they set the total measurement time to be equal, and optimized other parameters within that restriction. Also, optics was similar for all: fiber-optical probe with external light source.

Tables below summarize the results. Interestingly, the MEMS FPI (Spectral Engines' sensor) outperformed the wider range MEMS FTIR and grating instruments in moisture measurement and was equal to the grating spectrometer with cooled detector in polyethylene measurements. In both cases, the error was 20 times smaller than that of the MEMS FTIR. This can be mostly explained by the high throughput of the MEMS FPI, as a result of the off-plane configuration like explained in the previous sections, leading to higher SNR and shorter measurement times. In the pharmaceutical blends the MEMS FPI and the grating spectrometer produced very similar results, with linear array being slightly better. This demonstrates well that the end performance is not always straightforward to forecast from technology specifications only, and not even from one application to another!

Spectrometer	Polyethylene 2-σ error [g/m²]	Moisture 2-σ error [weight-%]
Micro FTIR	0.44	0.100
Micro FPI	0.02	0.005
Linear Array	0.01	0.017

Error of achieved application results for polyethylene thickness and moisture content.

Spectrometer	Paracetamol RMSEP [weight-%]	Lactose RMSEP [weight-%]	Microcrystalline cellulose RMSEP [weight-%]
Micro FPI	2.12	3.45	2.20
Linear Array	2.10	2.69	1.79

Error of achieved application results for pharmaceutical blends.

Another practical example is the EU Horizon Foodscanner Prize. This prize was set up to motivate companies and communities to build a device that can measure the nutrition values in food, allergens and potential harmful residues. The idea was to get new tools to the fight against obesity, diabetes etc. All top 3 finalists represented the (V)NIR spectroscopy technology, showing the power of the method. The finalists were Spectral Engines (MEMS FPI), TellSpec (grating with Texas Instruments' DMD) and Consumer Physics (VNIR multichannel). 50 unknown food substances were measured and a 15-person panel reviewed the technologies and the solutions. Finally, Spectral Engines was selected as the winner of the main prize of 800 000€, demonstrating once again the power of their MEMS FPI –based sensor technology.

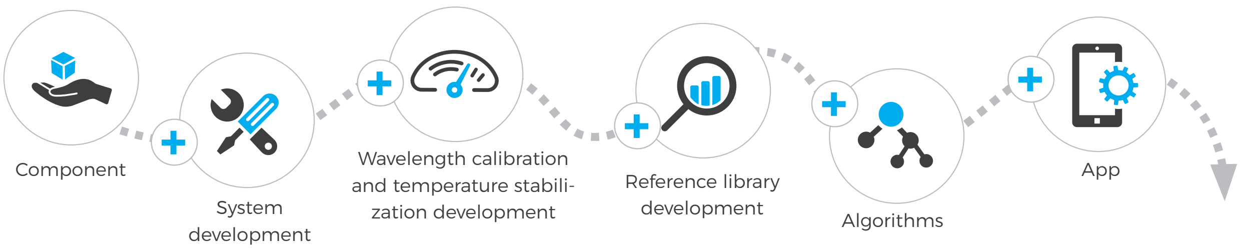
Usually it really is the application that decides which technology suits the best. There are some basic criteria for selecting the right platform for you without even going to the technical details of wavelength resolution etc. This selection logic is described in below, where you end up to the right platform by asking a few application and business-related questions. Once you have gone through this simple selection tool, it is much easier to narrow down your final selection, which then depends on the final specifications, cost targets and the level of solution (sub-component vs. full solution). This graph does not consider your business model which, naturally, is an important point.

	MEMS FPI	MEMS FTIR	LVF	Grating + DMD	NIR Grating	Monolithic NIR grating	VNIR grating / multi-channel
Reflection measurement							
Withstands harsh conditions							
Sensitive measurement							
Fast results							
Production capability for high volume							
Highly compact							
Specific measurement							
Ultra-low cost							
Very fast moving, heterogeneous sample							

High-level decision tree for an application and its business case.

Some companies provide only components, leaving system development, wavelength calibration and temperature stabilization development, along with the reference library and algorithm development to the customer, whereas others offer full end-solutions only. Most companies work between these two ends: for example Spectral Engines provides fully wavelength and temperature calibrated spectrometers including light sources (NIRONE Sensors), and for customers wanting to private label a solution and move to market quickly, the NIRONE Scanner platform provides the complete instrumentation, communication methods, cloud platform, reference library creation and algorithm implementation.

COMPONENT-BASED SOLUTIONS



EVERYTHING FROM ONE PLACE

Summary

Nowadays, there are plenty of technologies within NIR spectroscopy to choose from, as development is going fast towards smaller and cheaper devices. It is generally believed that NIR-based material sensors will appear in various industrial and consumer applications within this decade. Selecting the right platform for you needs some background research, but with a few main points to consider the options are already narrowed down.

The questions you want answers for are: do you want to buy components and invest in instrument and calibration development yourself, or do you want to get a ready-made platform, fitted to your application and gives you short time-to-market? Do you aim at high-volume market, a few special devices or something in between? Do you need especially shock and vibration resistant technology? Do you need to measure fast, or can you relax this requirement? How about connecting the devices to the cloud and performing analysis there?

After answering those top-level questions first, you can start getting in the details of comparing spectrometers. Finally, if you are selecting a platform, you need to evaluate the future of the platform, too - can this be made even smaller and cheaper or is this the limit? We at Spectral Engines are committed to continuous development. If you are unsure about your recommended solutions, please contact our team.

With plenty of technologies to choose from, selecting the right platform might be a bit tricky. With some background research the options will quickly narrow down. Spectral Engines is committed to continuous development - contact us for your recommended solutions.

MAIN SOURCES:

- Antila, J., Tuohiniemi, M., Rissanen, A., Kantojärvi, U., Lahti, M., Viherkanto, K., Kaarre, M. and Malinen, J. 2014. MEMS- and MOEMS-Based Near-Infrared Spectrometers. Encyclopedia of Analytical Chemistry. 1–36.
- TEMATYS: Market and technology report "Miniature and Micro Spectrometers: End-user needs, Markets and Trends"
- Paaso et al., Microspectrometers for paper, plastic and pharmaceutical applications, 2017
- Webpages and datasheets of related companies

Meaningful intelligence!

Let us to help you to build your own scanner for future material-sensing needs!

Dr. Stefan Schwarzfischer
CEO
+49 176 242 61042
stefan.schwarzfischer@spectralengines.com

DR. Dominik Rabus
Sales Manager, Europe
+49 176 576 04173
dominik.rabus@spectralengines.com