# The ultimate guide to spectrometer integration

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Ibsen photonics

You are probably reading this guide because you have been tasked to integrate an optical diode-array spectrometer into an analytical instrument. Congratulations! You are starting an exciting and challenging journey that involves hundreds of small and large decisions and compromises. The intention of this guide is to help you make the right decisions along the way. Spectroscopy is a multi-disciplinary area that involves chemistry, physics, mechanics, optics, mathematics, software, and electronics, and nobody can be an expert in all of these fields. Therefore, this guide only assumes that you have a basic understanding of the above-mentioned subjects. So, you may want to skip certain chapters if you are already an expert in those fields.

We will take you through the basic decision steps needed when integrating a spectrometer into an instrument. The first chapter will introduce you to the basic concepts of spectroscopy. The next chapter briefly describes the options you must consider for the light source. Chapter 3 will help you choose the right spectrometer based on your requirements in terms of things like wavelength range, resolution, frame rate, cost, etc. We have devoted a complete chapter to the coupling of light into your spectrometer since this is an often-overlooked area that can have an enormous influence on your final product performance and cost.

We hope you enjoy reading this guide and that it will be helpful.

**- Thomas Rasmussen, Ibsen Photonics**

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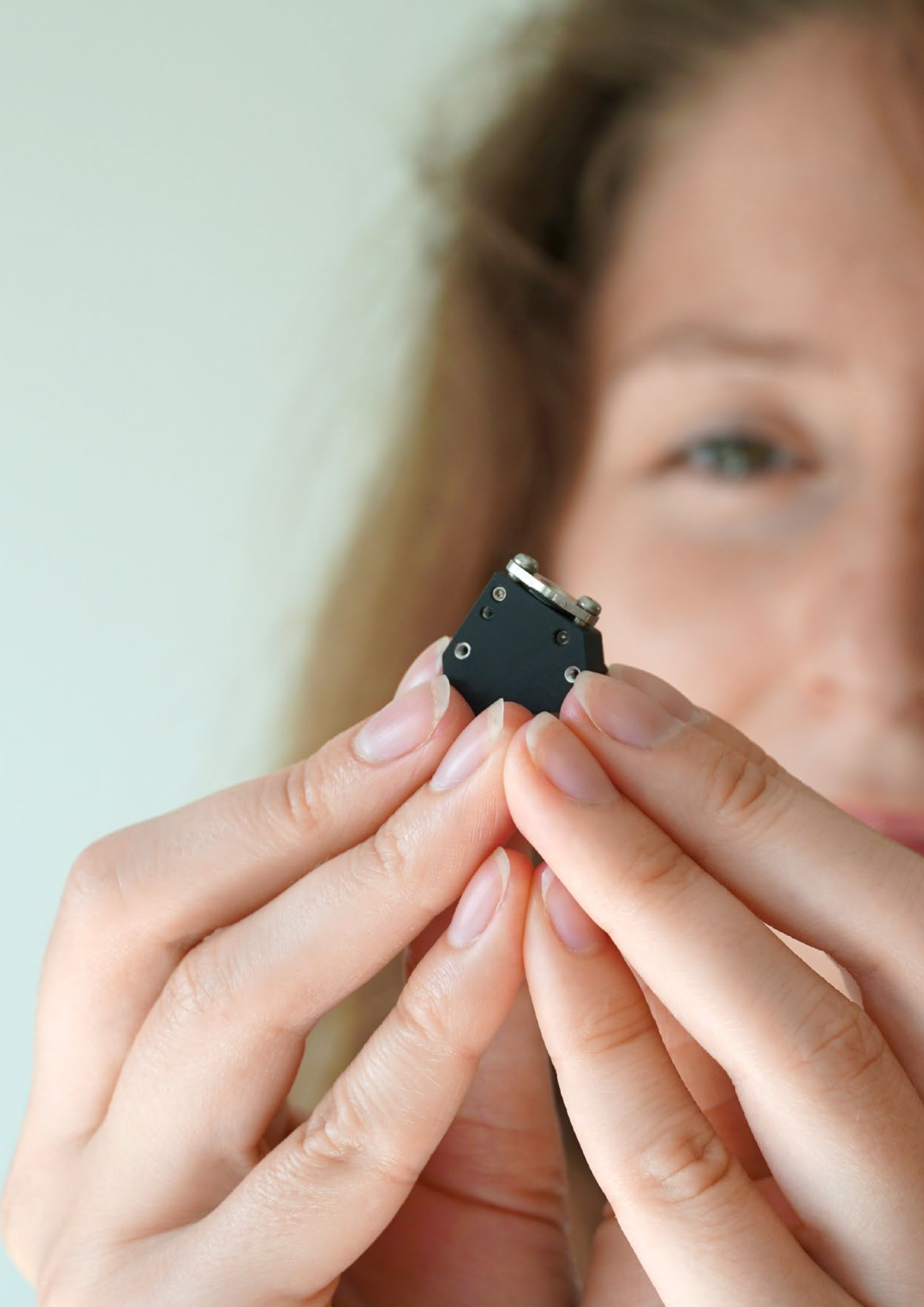


# Basic spectroscopy

Spectroscopy is used to identify and quantify the constituents of a sample. This can be the number of active ingredients in a pharmaceutical tablet, the protein content of the harvested grain, or the atomic content of a rock sample on Mars. There are many different techniques used for spectroscopy and in this guide, we limit ourselves to optical spectrometers typically used for molecular spectroscopy. This means that our instrument will use light to analyze the sample. As you may remember from your physics class in school, light can be described as electromagnetic waves with a wavelength – the distance between two wave tops – and a speed – the speed of light. Light is sub-divided by wavelength in regions named Ultra-Violet (UV), Visible (VIS), and Infra-Red (IR). The range between the VIS and IR is called the Near-IR (NIR). The human eye can only see the VIS range but we can use all ranges for spectroscopy. The main benefit of using light for spectroscopy is that it can provide fast (often real-time) results without destroying or interfering with the sample.


Figure 1: Optical Spectrum

A spectroscopic instrument records the spectrum being emitted from, reflected off, or transmitted through a sample. An example of an emitted spectrum is the light coming from the color screen of your mobile phone. The colors you see on the screen are constructed by mixing red, green, and blue light from a lot of small light sources inside the screen. When you have equal amounts of red green and blue our eyes see it as white light but, if we analyze it with a spectrometer we can clearly see the three distinct wavelength peaks as shown in Figure 2.

A spectroscopy instrument generally contains the basic elements shown in Figure 3 inside the dashed box. A light source to illuminate the sample, a spectrometer to record the spectrum, and a software model to convert the spectrum into useful information for the end-user.

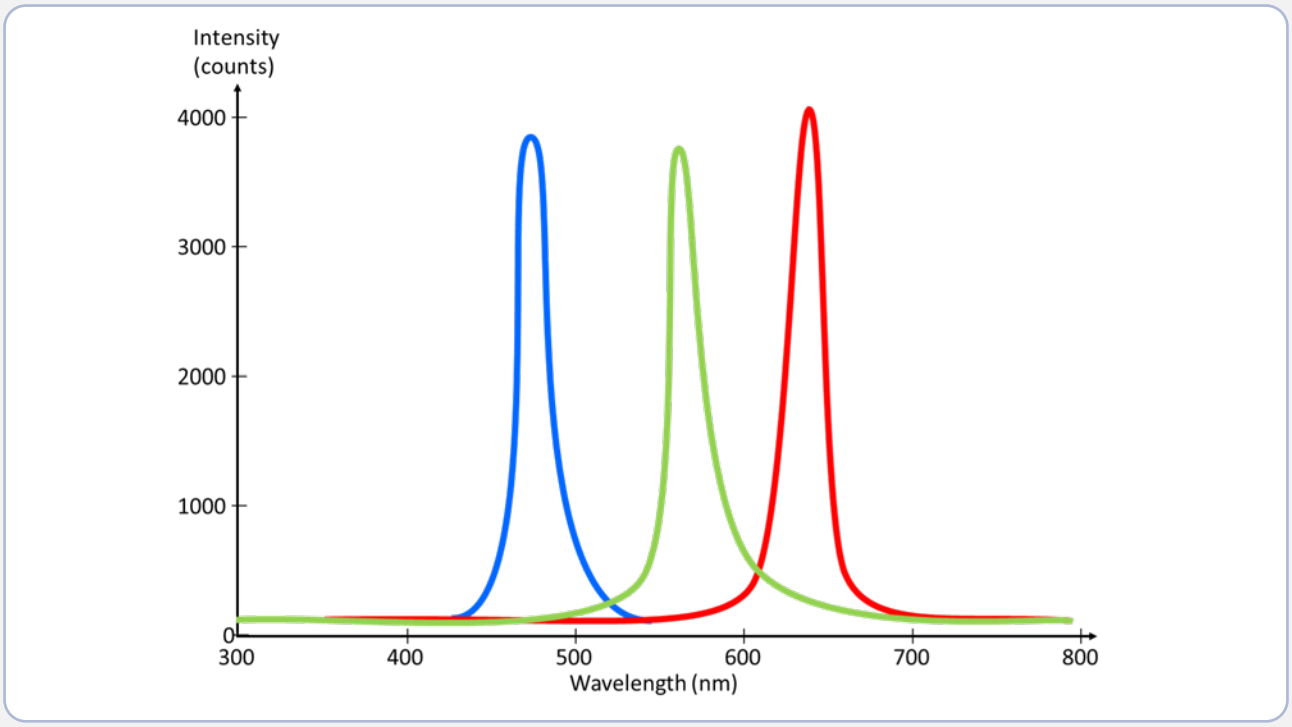



Figure 2: White light spectrum from mobile phone showing the three RGB color peaks.

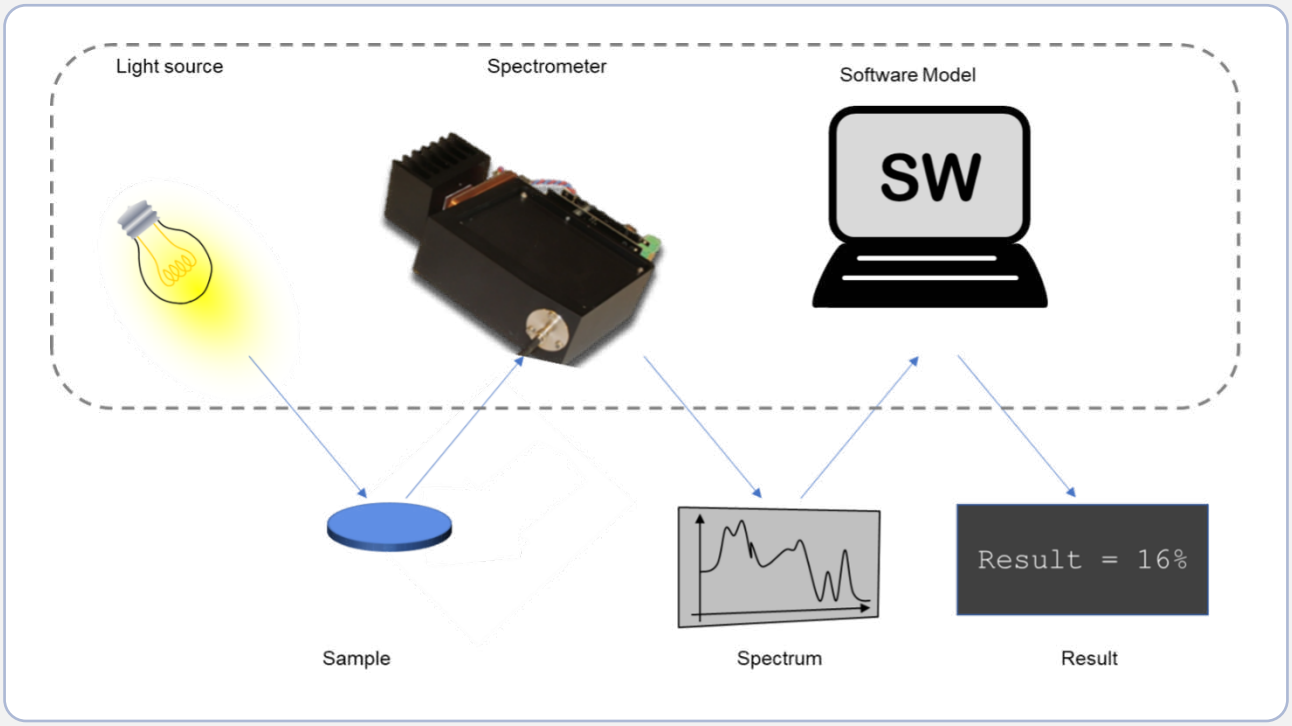



Figure 3: Basic building blocks of an analytical instrument. Light source to illuminate the sample, a spectrometer to record the spectrum, and a software model to convert the spectrum into useful results.

# Light source

There are many options for the light source but, your application will very often determine which type to use. In general, there are four categories of light sources:

## No light source required – the sample itself is the light source

This is typically the case when the sample itself emits light like the example of the spectrum of your mobile phone screen. So, if you are building a system to measure the spectrum of a display screen or a lamp you obviously don't need a light source in your instrument

## No light source required – the ambient light is used as a light source

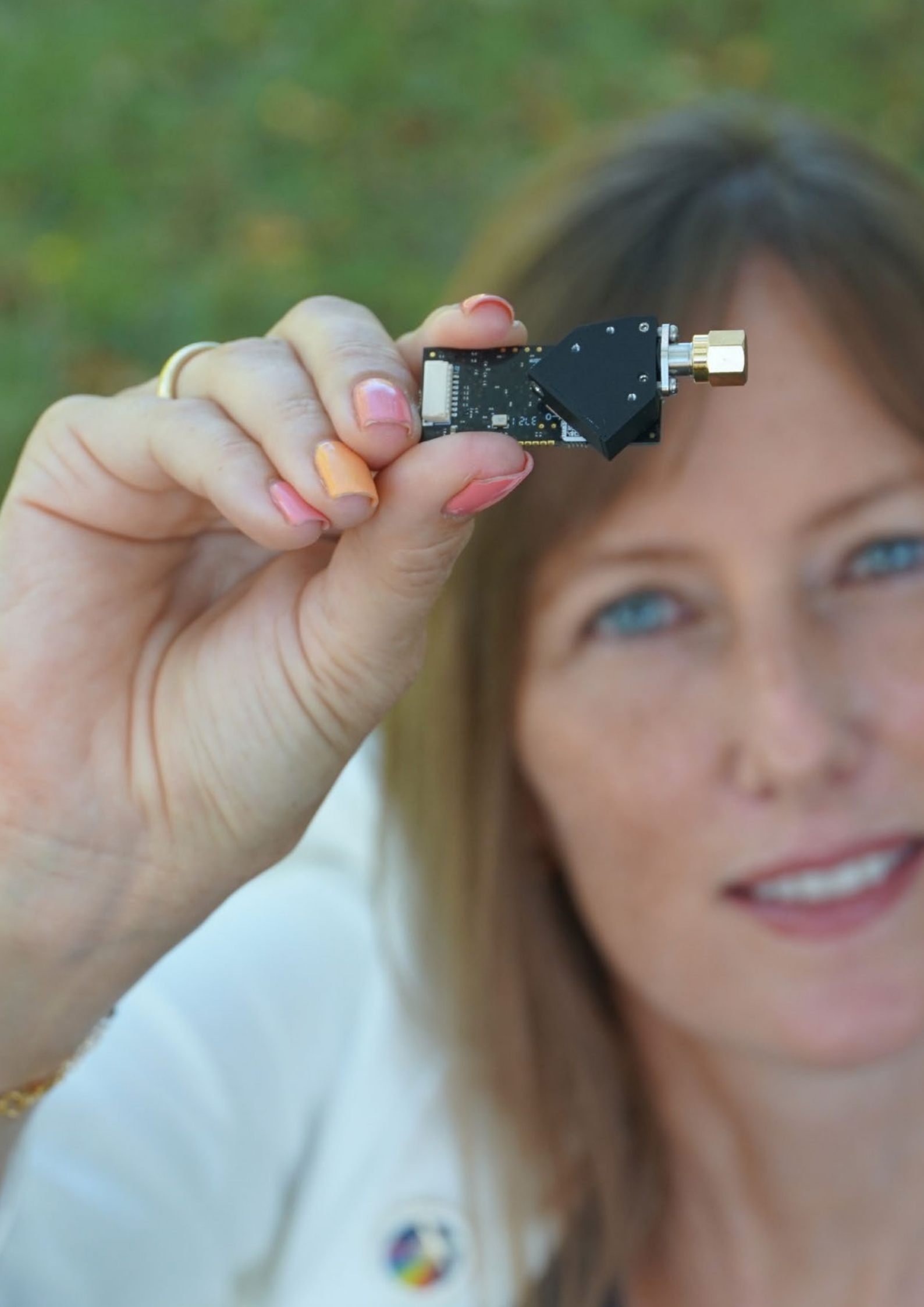
In some cases, you may be using the sun or the room lighting as your light source. An example is the monitoring of the reflection of sunlight in vegetation by spectrometers located on drones overflying the ground. In this case, you do not need to build in a light source in your instrument. However, you should bear in mind that both indoor lighting and especially the sun is a very variable light source, so your measurement method should be robust against large variations.

## Internal broadband light source

A broadband light source is required if you need to cover a large portion of the spectrum – typically several 100 nm. Broadband light sources are used extensively for absorption measurements in for instance UV-detectors for chromatography and near-infrared spectroscopy. Examples of common broadband light sources are Deuterium (UV), Tungsten/Halogen (VIS+NIR), and Xenon flash lamps (UV+VIS+NIR).

## Internal narrowband light source

If you are only concerned with a narrow part of the spectrum – typically less than 100 nm, then you can use Light Emitting Diodes (LED) which are very power efficient, compact, and low cost. LEDs typically cover between 10 – 50 nm. Some types of spectroscopy like fluorescence spectroscopy require a narrowband light source to illuminate the sample and the sample will emit at another wavelength. The same goes for Raman and Laser Induced Breakdown spectroscopy where an even narrower light source like a laser with less than 1 nm bandwidth is used.



# Spectrometer

The basic function of the spectrometer is to take the light input and detect the amount of light intensity at each relevant wavelength. This guide assumes you are going to work with a diode-array spectrometer (sometimes called a PDA or DDA).

## How a spectrometer works

The heart of the spectrometer is the diffraction grating which is the component that splits different wavelengths into different angles. This is illustrated in Figure 4 by the red, green, and blue wavelengths following different angles after the grating.

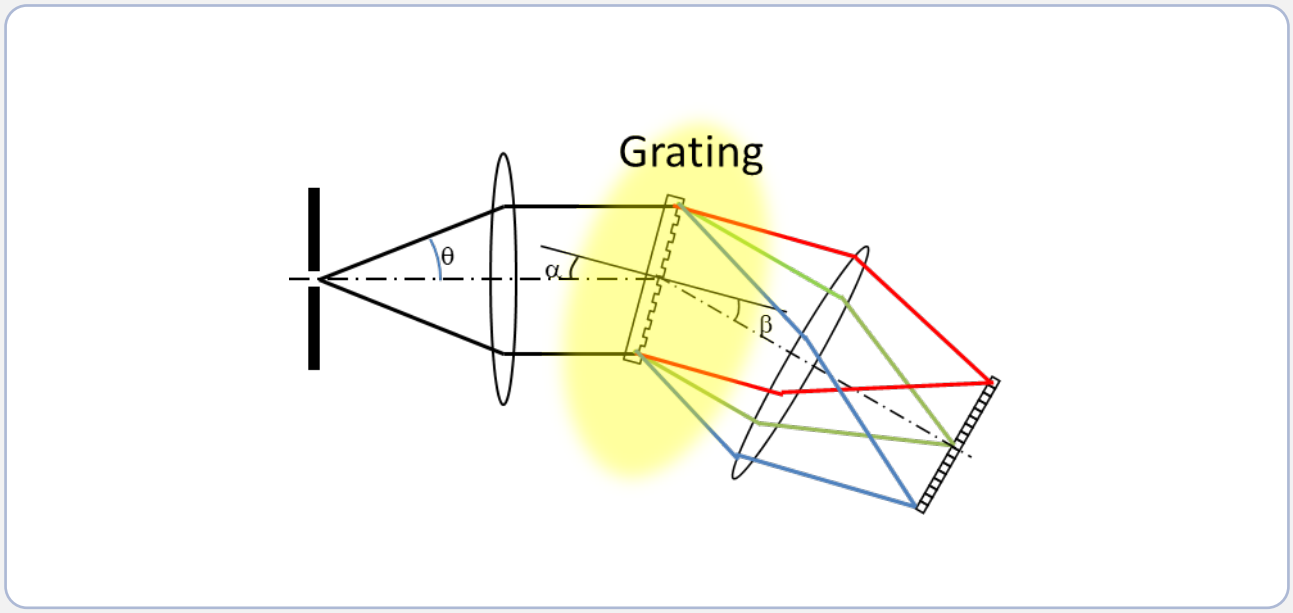



Figure 4: The grating is the wavelength selective element in the spectrometer.

For the grating to function properly we must ensure that the light hitting the grating is a parallel beam of light (so-called collimated light) for all wavelengths. This is ensured by placing a collimation lens in front of the grating and with a small aperture (called a slit) located in the focal plane of the collimation lens.

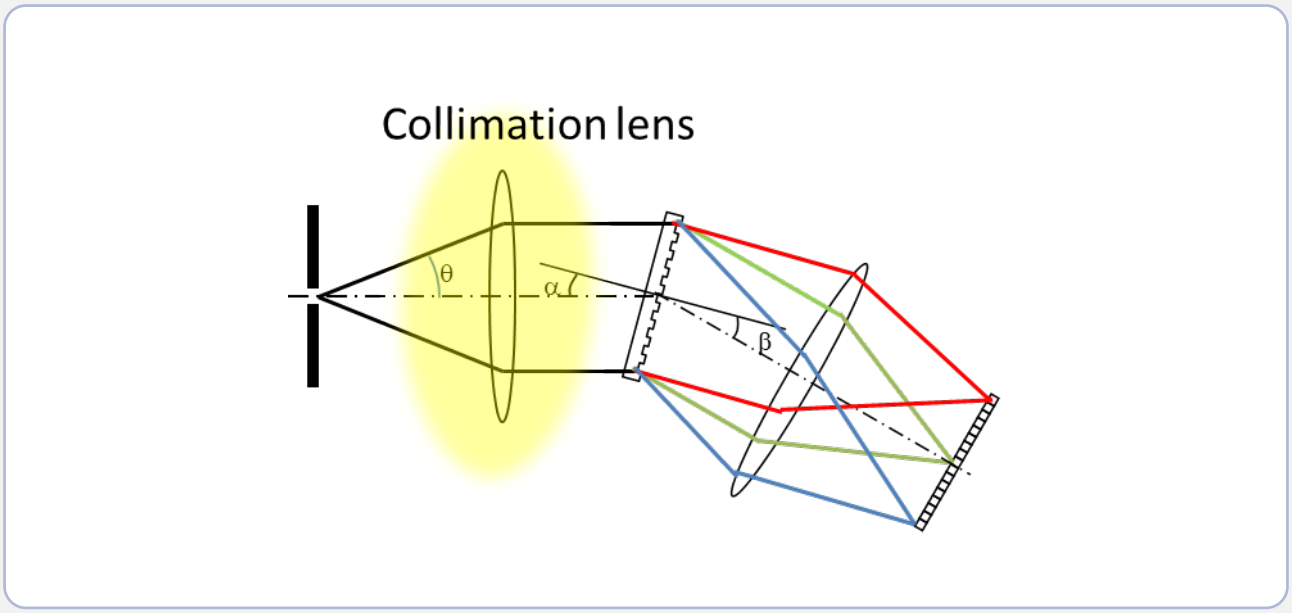



Figure 5: The collimation lens and the slit ensure that all wavelengths hit the grating at the same angle of incidence.

The slit at the entrance of the spectrometer has a dual function. As mentioned above it works together with the collimation lens to create collimated light. But, in most spectrometers, the slit also determines the resolution of the spectrometer. We will describe resolution later but, for now, let us just say that the resolution is the spectrometer's ability to distinguish one wavelength from another. The wider the slit the more the different wavelengths will be blurred and overlap and thus the poorer the resolution.

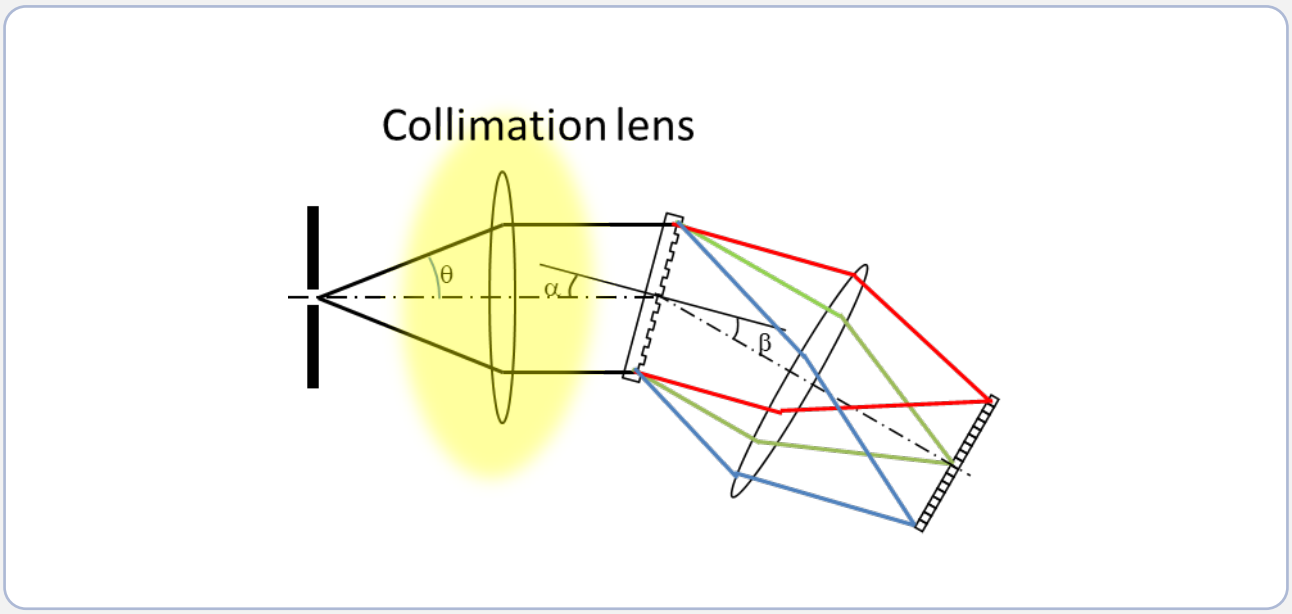



Figure 6: The slit determines the resolution of the spectrometer.

On the other side of the grating, we have a focusing lens whose function is to convert angle to position. Since the grating has split the different wavelengths up into different angles the focusing lens will focus these different wavelengths onto different positions in the focal plane of the Focus lens.

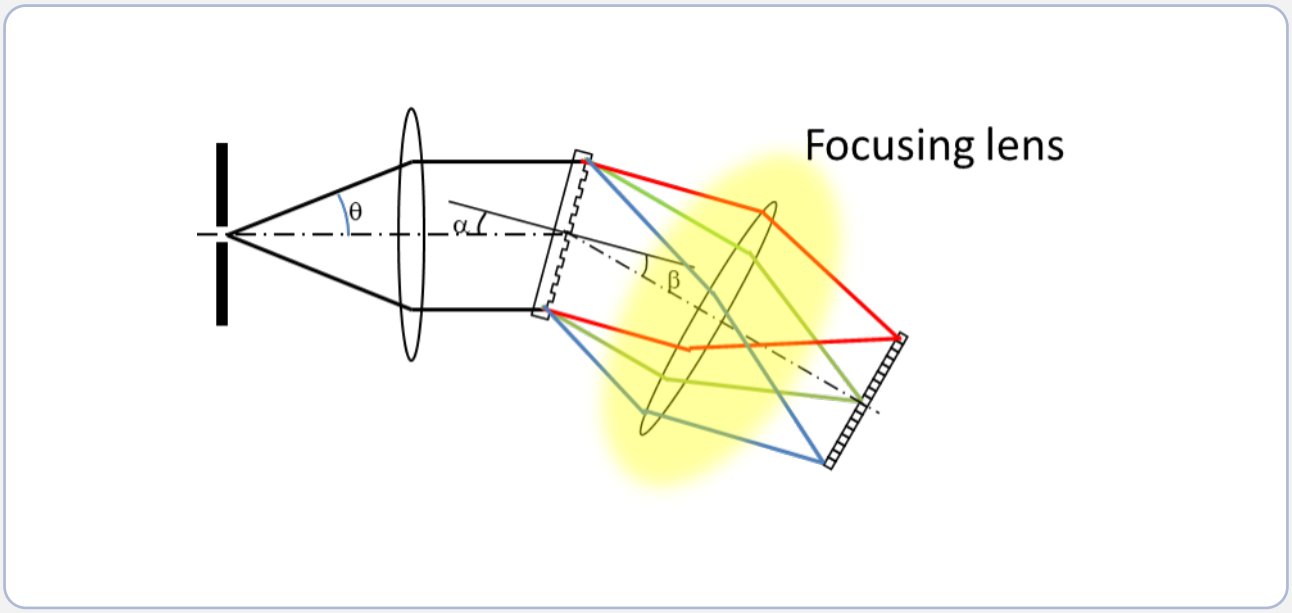



Figure 7: The focus lens focuses the different wavelengths on different locations in the focal plane.

And, in the focal plane, we place our diode array detector which is an array of small photo-detectors that convert light into an electrical signal (like a voltage or current). So, if your light input only contains blue light, we will get a strong electrical signal from the bottom detector in the array in Figure 8. However, if your input light contains only a red wavelength, it will be the topmost detector in the array that will have a strong electrical signal.

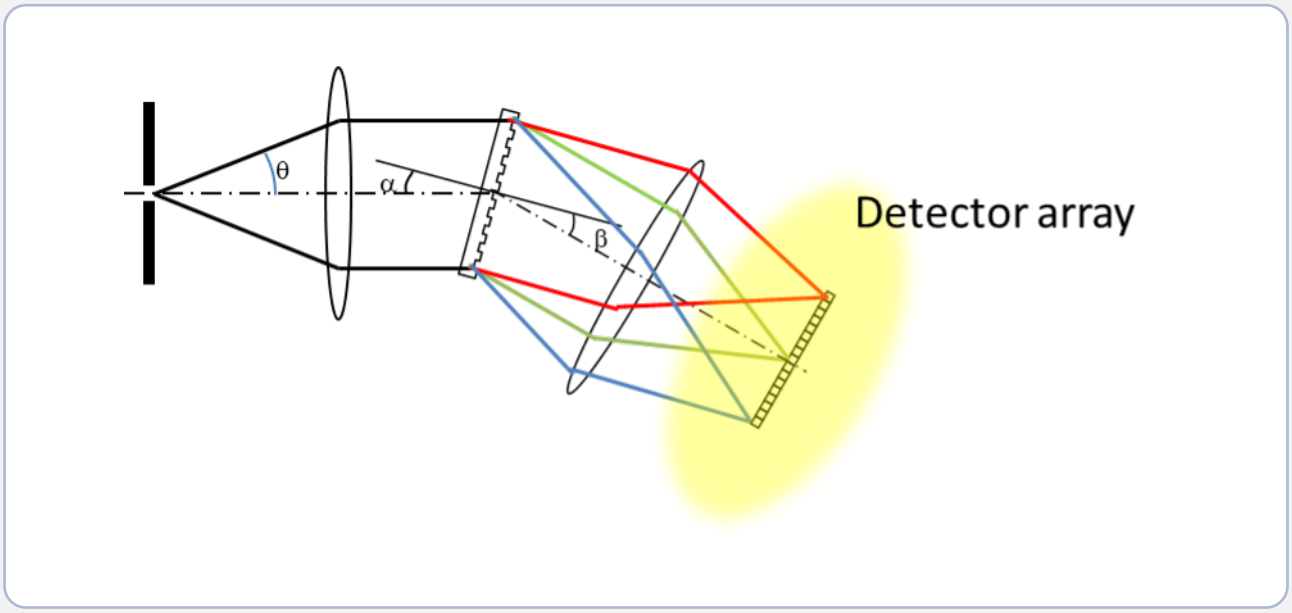



Figure 8: The detector array detects the intensity of the different wavelengths.

## Basic parameters

The key parameters to consider for your choice of a spectrometer are the wavelength range and resolution.

### Wavelength range

The wavelength range is simply the range of wavelengths that you need to cover. Let us say you want to analyze color, then you need to detect the visible spectrum from ca. 400 – 750 nm.

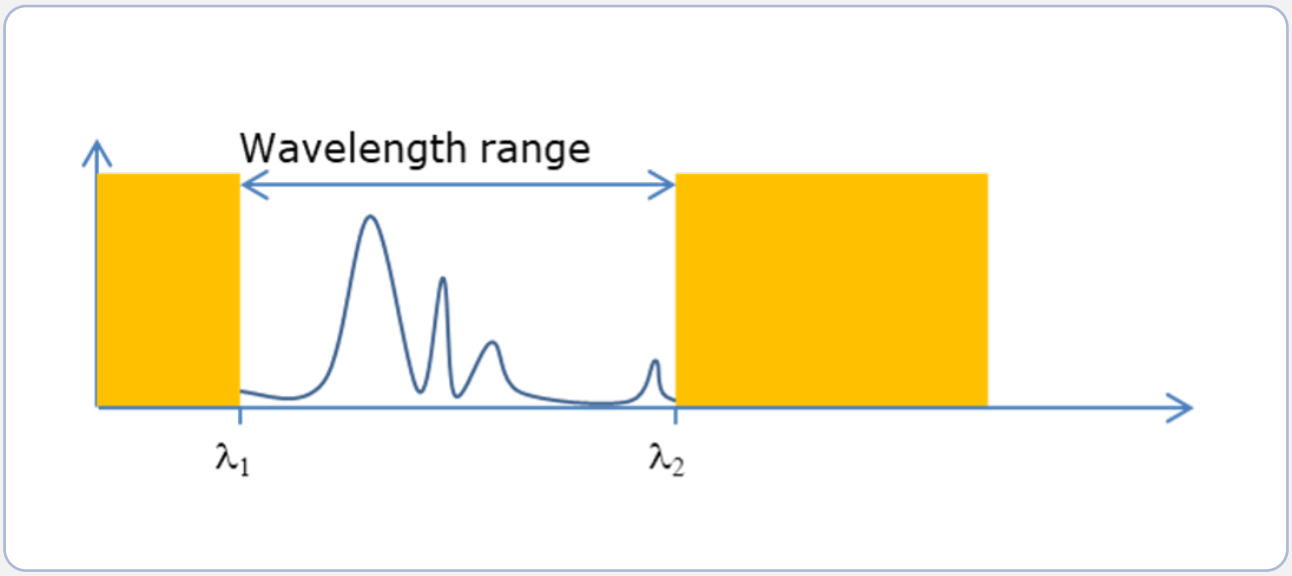



Figure 9: Definition of wavelength range.

### Resolution

The resolution is the spectrometer's ability to distinguish between different wavelengths. The term resolution can unfortunately have several meanings in spectroscopy dependent on the context. Especially three terms are often confused 1) pixel resolution, 2) optical resolution, and 3) spectrometer resolution. The pixel resolution is simply a measure of how well you sample your spectrum. If you are measuring from 400 – 500 nm with 100 pixels, your pixel resolution is simply (500 – 400 nm)/100 pixels = 1 nm/pixel. The optical resolution is the theoretical resolution of the spectrometer if you had infinitely many small pixels. And finally, the spectrometer resolution is the actual resolution of the spectrometer taking both the pixel and optical resolution into account. The spectrometer resolution is normally the only resolution parameter you need to worry about.

In Figure 10, we have illustrated the importance of resolution. To the left we have plotted the light input to the spectrometer which is two individual single wavelengths – this could be lines from a fluorescent lamp as an example. The fact that the spectrometer has a finite resolution means that these spectral lines will be broadened by the spectrometer. The middle plot shows a situation where the spectrometer resolution is okay. The two lines are broadened as expected but not more than we can still clearly see that there are two individual wavelengths and we would be able to determine their center wavelengths with quite a good accuracy. The right-most plot, however, shows a situation where the resolution is too poor. The two peaks completely overlap and when we look at the overall spectrum there is no way we can tell that originally there were two peaks.

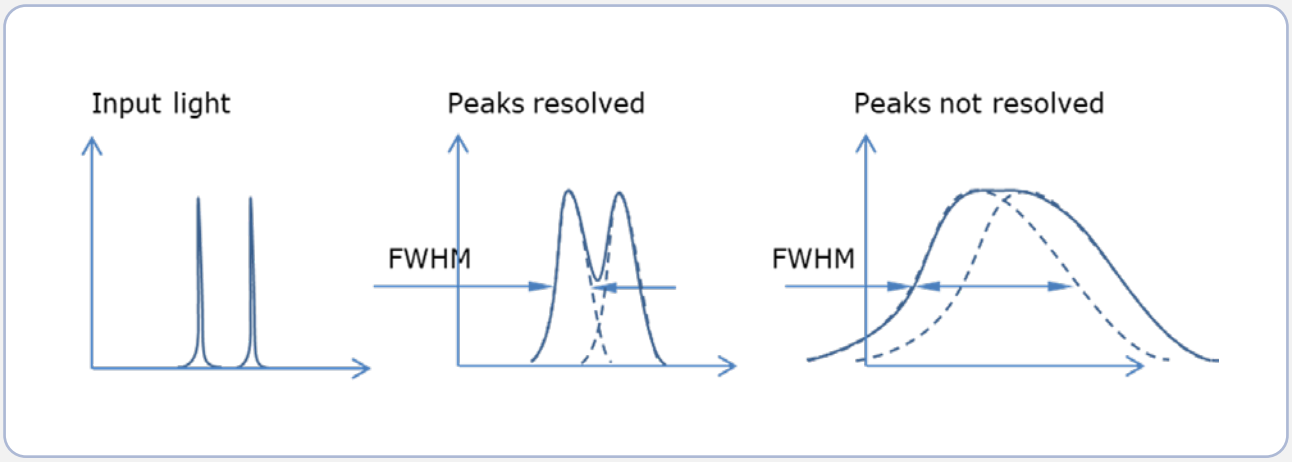



Figure 10: Influence of resolution of the spectrometer. Leftmost graph: Input light, Center graph: spectrometer with adequate resolution, Rightmost graph: Spectrometer with too poor resolution.

As mentioned earlier, the resolution is in most cases determined by the slit width. So, in order to obtain a high resolution (low numerical value for the resolution in nm), you want to choose a narrow slit. However, the slit is also limiting the amount of light you can couple into your spectrometer. Therefore, you should always work with the largest possible slit width that will fulfill your resolution requirements.

### Choice of slit width

- ✔ Always use the widest possible slit width that fulfills your resolution requirement

## Size

The size of a spectrometer is driven mainly by the focal lengths of the optics used. The focal length ( $L_F$ ) of a spectrometer is related to the detector length ( $L_D$ ), the grating groove density ( $G$ ), the wavelength range ( $\lambda_2 - \lambda_1$ ), and the diffraction angle ( $\beta$ ) by the following approximate equation:

$$L_F = \frac{L_D \cos(\beta)}{G(\lambda_2 - \lambda_1)}$$

From this equation it is clear that a compact spectrometer can be obtained with the following methods:

**Compact spectrometer**

- ✔ Choose a grating with a high groove density
- ✔ Choose a short detector

Unfortunately, these parameters cannot be chosen arbitrarily as we will describe in the following.

## Maximum Grating Groove density

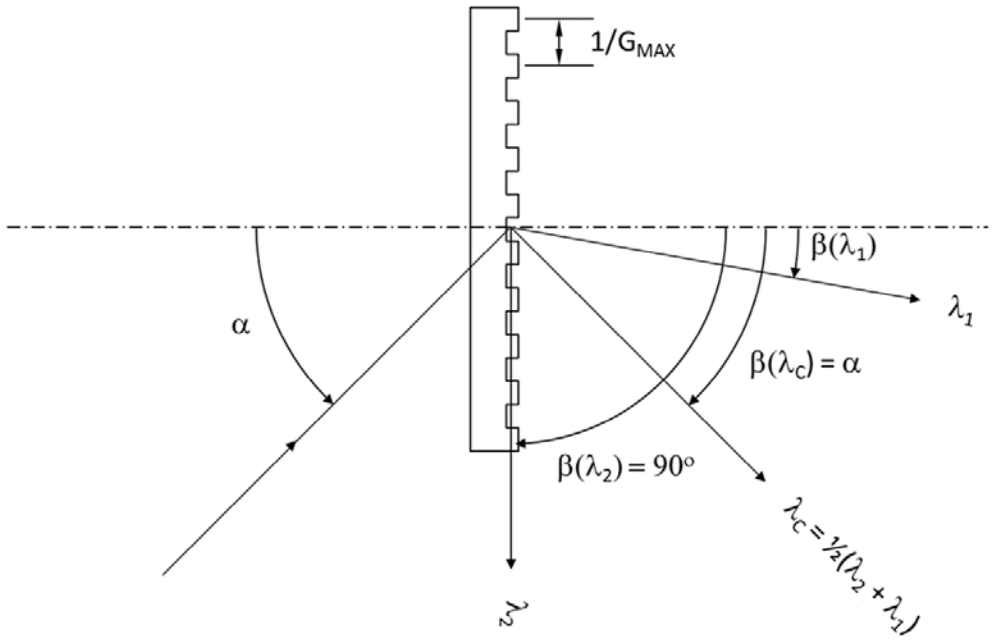



Figure 11: Illustration of maximum grating groove density for wavelength $\lambda_2$.

The function of the grating is to diffract (bend) the incoming light by different angles depending on the wavelength. The diffraction angle increases with wavelength and once the diffraction angle reaches 90 degrees relative to the normal of the grating for the longest wavelength ( $\lambda_2$ ), the grating is no longer working for this wavelength. In this way we can obtain a simple formula for the theoretical maximum groove density ( $G_{MAX}$ ) for a given wavelength range as follows:

$$G_{MAX} = \frac{4}{3\lambda_2 - \lambda_1}$$

In practical cases, you should likely stay at 90-95 % of the maximum groove density.

### Example of maximum grating groove density:

You want your spectrometer to cover 800 – 1100 nm. Then the theoretical maximum groove density you can use is 1600 lines/mm. you should likely not use a grating with more than 1500 lines per mm.

## Minimum detector length

The detector length will in most cases be limited by the resolution you want your spectrometer to resolve. If we define that the detector consists of ( $N$ )pixels with a pixel-to-pixel spacing of ( $w$ ), then the detector length ( $L_D$ ) is:

$$L_D = Nw$$

The smallest pixel spacing of most scientific detectors is typically 7 - 10 microns. As a rule of thumb, the FWHM resolution peak ( $\Delta\lambda_{FWHM}$ ) should be sampled by 2 – 3 pixels. So, if we use 2.5 pixels we can estimate the minimum required detector length as:

$$L_{D,MIN} = 2.5w\frac{(\lambda_2 - \lambda_1)}{\Delta\lambda_{FWHM}}$$

### Example of minimum detector width:

You want your spectrometer to cover 800 – 1100 nm with a resolution of 0.4 nm. The detector pixel width is 7 microns which means the smallest possible detector length you can use is 13.125 mm.

# Cost

The main cost drivers in any spectrometer are the number and size of the optical components and the choice of detector.

## Size of optical components

The graph in Figure 12 is made by plotting the cost of standard lenses from a lens supplier's catalog as a function of the diameter of the lenses.

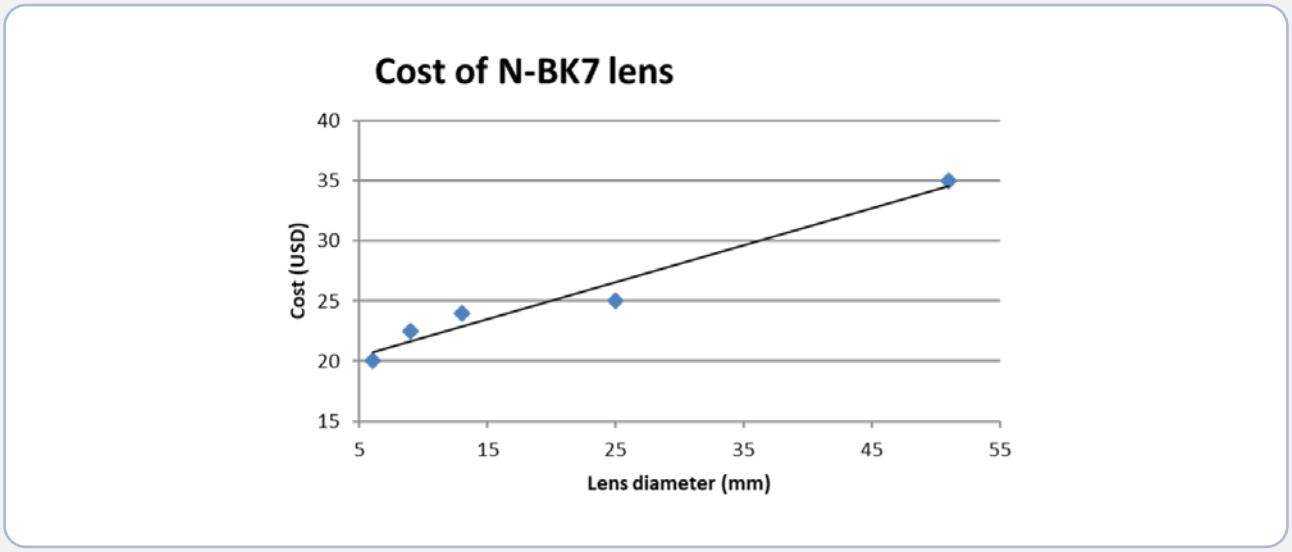



Figure 12: Cost of commercial lenses versus lens diameter.

It is obvious that the cost of the lenses increases more or less linearly with the diameter of the lenses.

## Detector choice

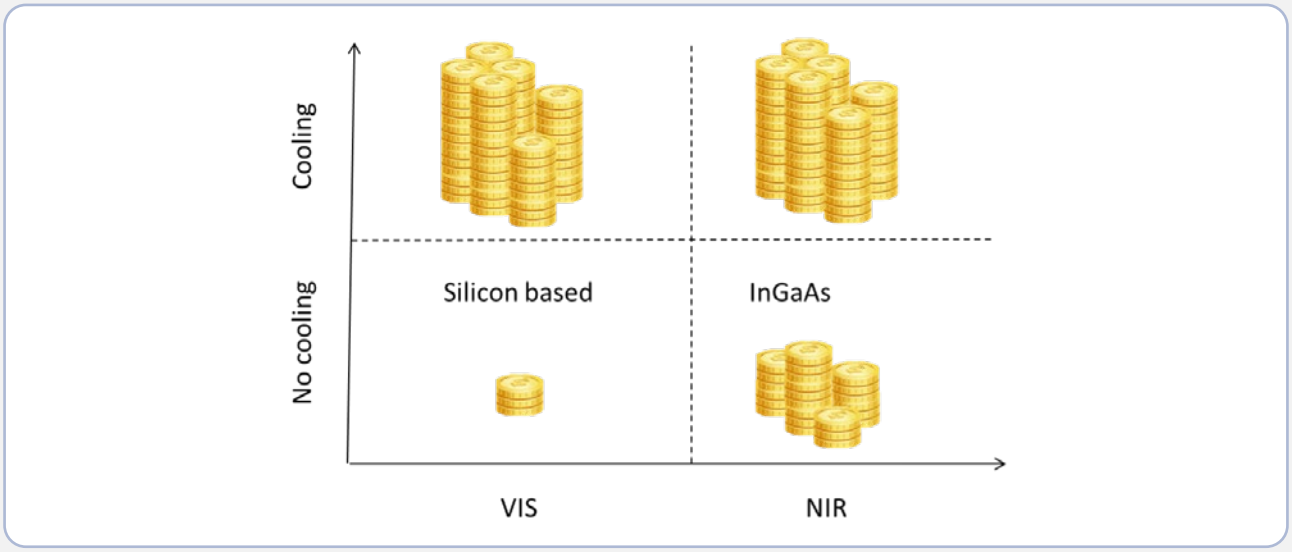



Figure 13: Relative cost of cooled and non-cooled silicon and InGaAs-based detectors.

The detector used inside the spectrometer can cost from a few EUR to thousands of EUR depending on mainly three factors:

- Wavelength range
- Cooling
- Speed

The wavelength range basically determines which detector material can be used. The lowest cost option is silicon which works well as a detector from UV (~175 nm) to around 1100 nm. Above 1100 nm Silicon is transparent and other (more expensive) materials like for instance InGaAs must be used.

If the detector needs to be cooled the cost is also considerably higher than for a non-cooled detector. The reason is mainly, that the thermoelectric cooler needs to be integrated into the chip, and the housing needs to be hermetically sealed and filled with an inert gas to avoid condensation.

Finally, if the detector array must be read very quickly – for instance reading 2048 pixels with a rate of 100 kHz - the detector and accompanying electronics tend to be expensive.

**Low cost spectrometer**

- Use a few small optical components
- Work below 1100 nm
- Avoid cooling the detector
- Avoid very fast frame rates

## Speed

The speed of a spectrometer is measured as the number of spectra that can be read per second – often termed the frame rate. An example of an application that requires a fast frame rate is the analysis of items on a conveyor belt that passes by the spectrometer at a certain speed. If the conveyor belt is moving with say 2 meters/sec and the spectrometer should measure a spectrum for every cm, then you need the spectrometer to read out 200 frames per second.

Three parameters determine the frame rate of a spectrometer:

- Detector chip clock rate
- Read-out circuitry / Camera electronics
- Throughput of spectrometer

### Detector chip clock rate

A diode array detector consists of a large number of pixels that each convert incoming light intensity (photons) to electronic charge (electrons). Once a strong signal (many electrons) has been built the pixels are read out one by one. The time it takes to read out all pixels represents the theoretically shortest time between each spectrum and thereby the fastest possible frame rate. The data sheet of a diode array detector will often tell either the maximum clock frequency or the maximum frame rate.

#### Example of frame rate limited by detector clock frequency:

Assume we want to use a detector with 2,048 pixels and a maximum clock frequency of 10 MHz.

In that case we can calculate the maximum frame rate as:

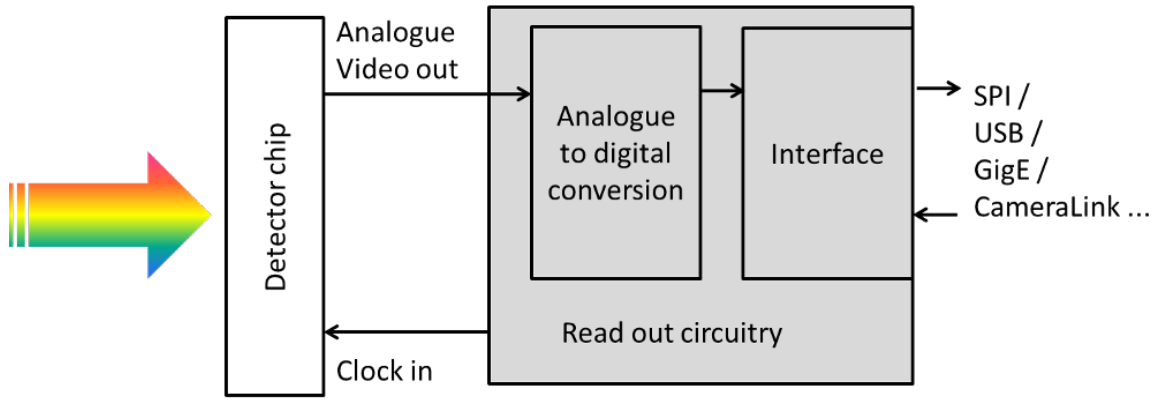
Maximum frame rate = 10,000,000 Hz / 2,048 pixel = 4,800 Hz

In general, diode arrays based on Charge Coupled Devices (CCDs) are slow (< 1kHz for 2,048 pixels) and diode arrays based on Complementary Metal Oxide Sensors (CMOS ) are fast (>1kHz for 2,048 pixels).

### Read-out circuitry

As mentioned in the previous section, the electron charge of the pixels in the diode array is read out in serial. The circuitry performing this operation is the read-out circuitry and has two basic functions as shown in Figure 14:

- convert the analog voltage levels from the detector chip to a much more robust digital signal
- package the digital data in a standardized format that a microprocessor or computer can use (like a USB port).




The read-out circuitry will also have a maximum frame rate that it can operate at and this is in most cases the limiting factor to your overall spectrometer speed. The read-out frame rate depends on three parameters; the interface clock frequency, the bit depth (the number of bits used in the A/D converter), and the number of pixels.

Obviously, the faster the interface clock frequency the faster the frame rate but, as seen from the above equation, you can also increase the frame rate by reading out fewer pixels and/or reducing the number of bits. See the table below for examples of how the number of pixels and bit depth can dramatically change the frame rate.

$$Frame\ Rate = \frac{Interface\ clock\ frequency}{Bit\ depth\ x\ number\ of\ pixels}$$

However, decreasing the number of pixels means decreasing the spectral resolution, and decreasing the bit depth decreases intensity resolution. If the maximum intensity the spectrometer can measure is 1,000 W/m2, then we can measure differences in intensity of 0.01 W/ m2 with a 16-bit A/D converter but only differences of 1 W/ m2 with a 10-bit A/D converter.

### Example of frame rate with different bit depths and number of pixels:

| | | | |
|---|---|---|---|
| Interface clock frequency | 25 MHz | 25 MHz | 25 MHz |
| Number of pixels | 2,048 | 256 | 256 |
| Bit depth | 16 | 16 | 10 |
| Frame rate | 0.7 kHz | 6 kHz | 10 kHz |

## Spectrometer throughput

The spectrometer throughput should ideally be 100% in which case all the light that enters the spectrometer ends up at the detector. However, in practical spectrometers, the throughput can be quite low due to losses in optical components and cropping of the light by apertures. If the signal that reaches the diode array detector is very weak we need to increase the integration time in order to build a strong signal. But, when we integrate over a long time we cannot obtain a fast frame rate. If for instance, the integration time is 100 milliseconds, then we can maximally read out 10 spectra per second even if the detector and read-out circuitry might allow much faster speed. Therefore, in order to obtain a fast frame rate, we want to use a spectrometer with the highest possible throughput – or lowest possible optical loss.

### High speed spectrometer

- ✓ Use a detector chip with a high clock frequency
- ✓ Use a read-out circuitry with a high interface clock frequency
- ✓ Use few pixels
- ✓ Use low bit depth
- ✓ Use a sensitive spectrometer

## Synchronization

Some types of measurements require the spectrometer to be synchronized with a certain trigger. One example is if your light source is pulsed with a short pulse – such as Xenon flash lamps that have pulse widths of a few microseconds and typical repetition rates in the 100 Hz range. Another example is if your sample is moving relative to the spectrometer and light source – like when the sample is on a conveyer belt or a carousel.

In the abovementioned cases, the start and stop of the integration time must be precisely synchronized with either the light source pulses or the location of the sample. Typically, there will be an electrical signal available that you can use to trigger the start of the integration time of the spectrometer.

If you need your spectrometer to support precise synchronization you must select the right type of detector and electronics. In general CCD's are not suitable for accurate synchronization unless they have a built-in shutter. In contrast, CMOS sensors and InGaAs sensors support by nature very accurate synchronization.

Furthermore, it is important that your electronics is capable of accurate timing with low jitter. As a general rule, it is better to use hardware based timing (with for instance Field Programmable Gate Arrays, FPGAs) than software controlled timing (using for instance micro-processors).

### Spectrometers with accurate synchronization

- ✔ Use detector chip with build-in shutter
- ✔ Use read-out circuitry with hardware-based timing

## Sensitivity

The sensitivity of a spectrometer is a measure of how well the input optical signal is converted into a strong electrical signal – typical a voltage or current level. There are basically three factors that influence the overall sensitivity:

- The throughput of the optical system from the input slit to the surface of the detector
- The conversion from photons to electrons of the detector chip
- The maximum amount of integration time

### Throughput of the spectrometer

#### Etendue

Ideally, the throughput of a well-designed spectrometer should be limited by the area and numerical aperture of the detector. The maximum amount of optical energy that the detector can accept is given by the so-called etendue, which is calculated as the detector pixel area times the numerical aperture squared:

$$Maximum\ Etendue = Area_{detector} NA^2_{detector} = Area_{detector} \sin^2(\theta_{detector})$$

See the figure below for the definitions.

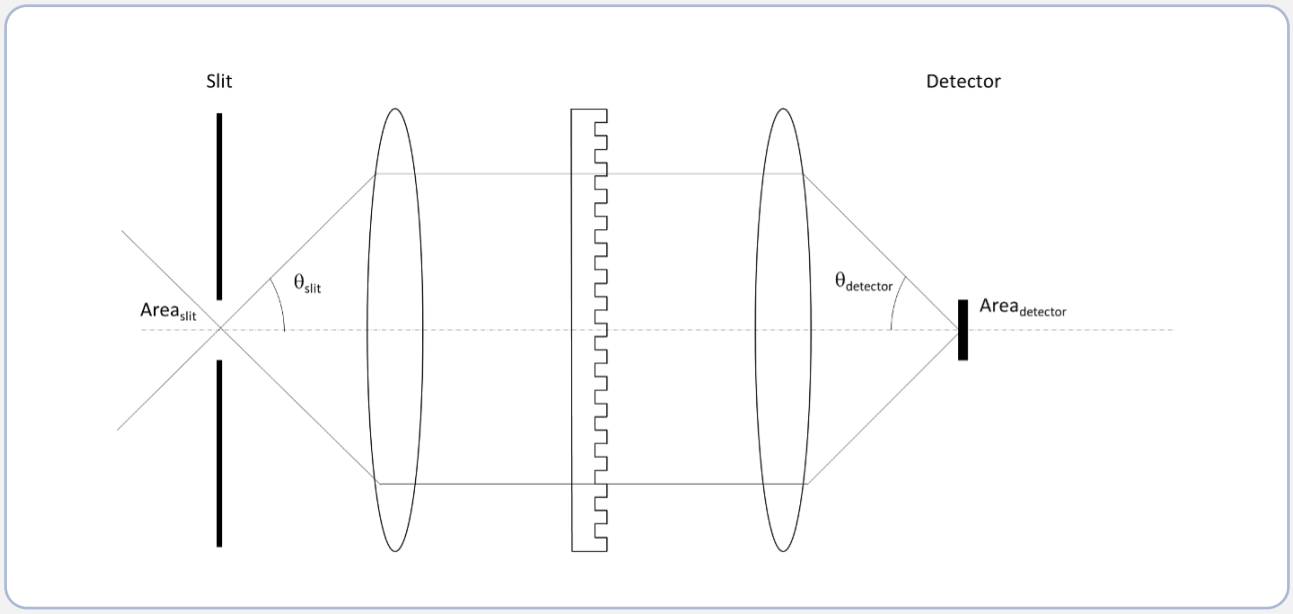



Figure 15: Definition of Area and numerical aperture at the entrance (slit) of the spectrometer and the detector.

In order to avoid losses through the system, the various optical elements and apertures must preserve the etendue of the detector. Eventually, this means that a well-designed system should fulfill the following:

$$Area_{slit} NA_{slit}^2 = Area_{detector} NA_{detector}^2$$

Which simply states that the etendue at the entrance of the system should be identical to the etendue of the detector.

If the etendue at the entrance is larger than that of the detector, the excess input power will simply be lost at the detector. If the entrance etendue is smaller that of the detector, you are not using the full potential of the detector.

Most detectors actually accept light with a quite high NA. Designing a spectrometer with a high NA is possible, but it comes with a consequence. In general, high NA optical systems require complex lens systems which in turn make them expensive, large, and heavy. So, if you are looking for a compact and low cost spectrometer, you likely have to compromise on the NA and thereby on the maximum amount of input light the spectrometer can capture.

**Optical losses**

The optical components used in the spectrometer (lenses and mirrors) all contribute to a small loss of energy. Typically, good lenses with AR coating offer 98 – 99 % transmissivity per lens (i.e. only 1 – 2 % loss) whereas typical Aluminum-coated mirrors offer 90 % reflectivity (i.e. 10 % loss) per mirror. More advanced dielectric mirrors with 99 – 98 % reflectivity can however also be used.

Generally, you should use as few and as highly efficient optical components as possible to reduce optical losses. This rule might be conflicting with the desire to build a high NA spectrometer since a high NA spectrometer generally requires a lot of lenses. Consequently, a compromise between high NA and the number of lenses must be made.

## Diffraction grating

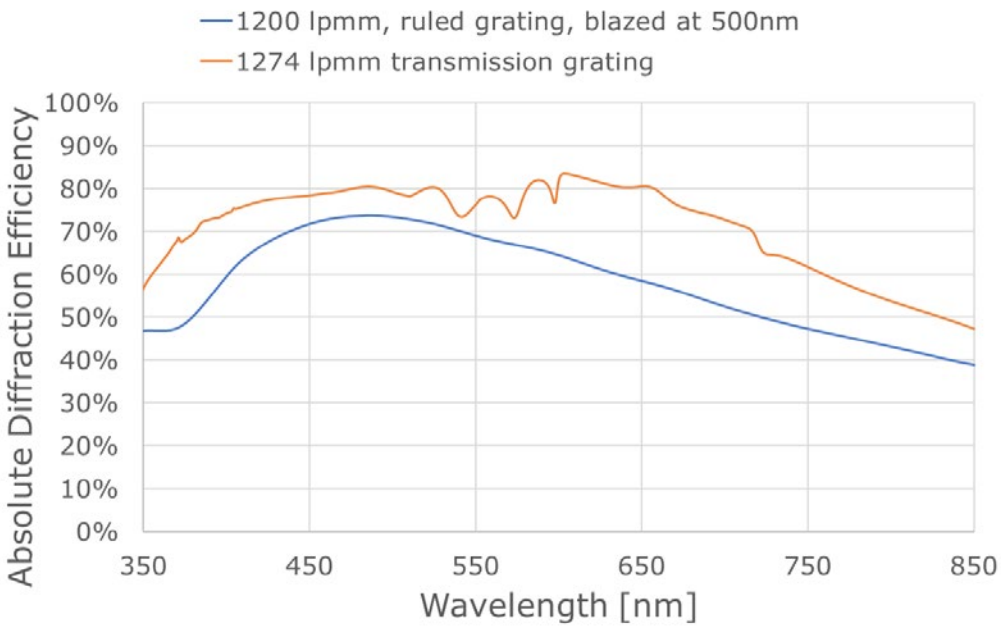



Figure 16: Comparison of the diffraction efficiency of a transmission grating and a reflection grating.

As mentioned in the introductory section on how a spectrometer works, the diffraction grating is the optical element that separates the different wavelengths of the spectrum into different angles. The efficiency of this diffraction depends on the wavelength and the physical structure of the grating. The most common type of grating in spectrometers is a ruled, Aluminum coated reflection grating, which has a triangular shaped grating tooth profile. The Aluminum coating itself has a reflectivity of 90 % and the ruled grating structure typically has 70 % efficiency at the best (blaze) wavelength but exhibits lower efficiency at shorter and longer wavelengths than the Blaze wavelength.

In contrast to reflection gratings, transmission gratings are phase gratings that are made in pure glass. Traditionally, transmission gratings have been considered low efficiency gratings but, during the past 20 years, this has changed. Modern transmission gratings can be designed to exhibit an almost flat high diffraction efficiency of 80 - 90 % over a rather wide wavelength range. See Figure 16 for an example.

As a rule of thumb, for the best efficiency, you should consider a transmission grating over a reflection grating.

### High throughput spectrometer

- ✔ Match the slit area and entrance numerical aperture to the detector
- ✔ Use as few and as low loss optical components as possible
- ✔ Use a transmission grating with high diffraction efficiency

## Photon to electron conversion

The function of the photo-detector is to convert light energy to an electrical signal (voltage or current level) and obviously the higher the conversion efficiency the better. Light can be described as particles called photons that each carry a small amount of energy. The photo-detector is typically made of a semi-conductor material (like Silicon) that will absorb the photons and convert their energy into electronic charges. The electronic charge can also be described as particles called electrons. Several factors contributes to the conversion from light energy to electronic charge and some are more important than others to maximize.

### Quantum Efficiency

Any detector will have a basic quantum efficiency (QE) which simply states the ratio between the number of generated electrons to the number of incoming photons. The QE cannot be larger than 100% and is often much less. The QE also depends on the wavelength. Naturally, you should choose a detector that has the highest possible QE in the wavelength region you are interested in.

### Pixel Well Depth

The well depth of the pixels of the diode array detector also has an influence on the sensitivity. The well depth is measured in electrons and tells how many electrons can be collected by the pixel before it is saturated. A small electron well will appear more sensitive than a deep well because the maximum signal (saturation) is reached with much fewer photons. However, it is important to note that the noise will be worse in a shallow well compared to a deep well. This can be understood by a simple example. In the case of a shallow well depth of say 100 electrons, one randomly generated (noise) electron will change the overall signal by 1% compared to the full well (100 electrons) signal. In a well depth of 100,000 electrons, however, one randomly generated electron will only change the overall signal level by 0.001%. A detector with a small pixel well will thus appear more sensitive, since the integration time until the maximum signal is shorter than for a detector with a deep pixel well. However, since the signal-to-noise ratio will be worse for the small well detector the actual choice of the detector will depend on whether sensitivity or noise is the most important factor in your application.

### Electronics Gain

Once our photons have been converted to an electric signal we can naturally amplify the signal using amplifier circuits. However, the amplifier will not only increase the signal level but also the noise level. This means that, if your signal is comparable with the random dark noise in the detector you will not benefit from amplification.

## Integration time and cooling

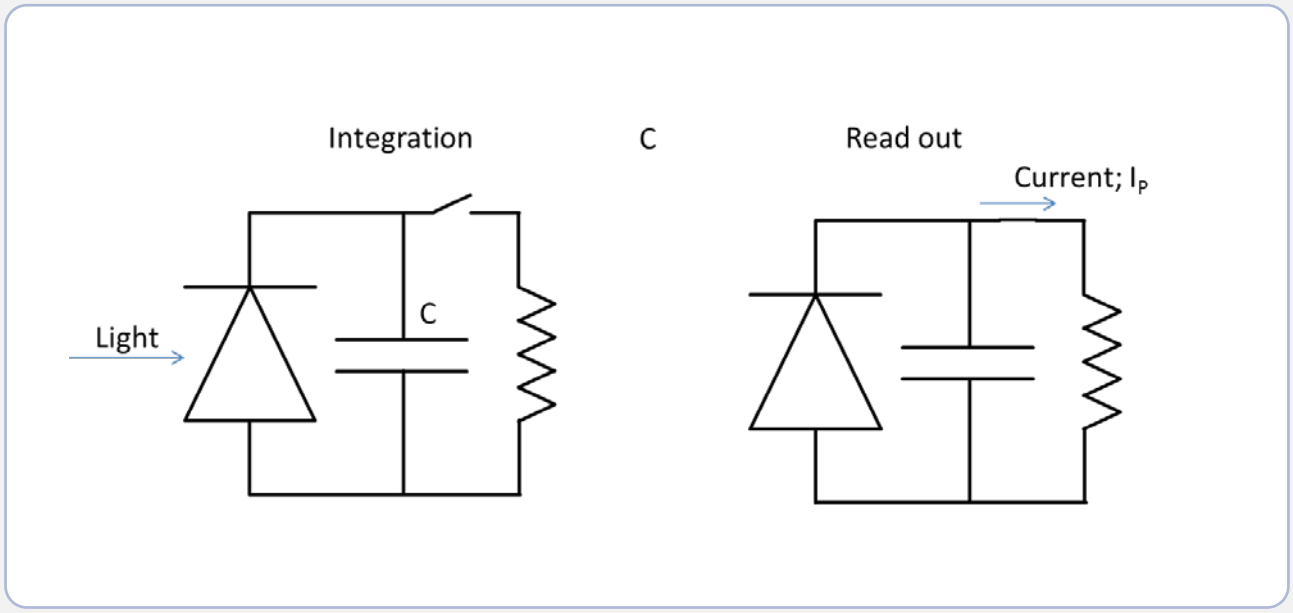



Figure 17: Electrical representation of detector pixels. Left: during integration, Right: during read-out.

In diode array spectrometers the detector is of the integrating type. The concept is illustrated in Figure 17 where each pixel is represented by a photodiode, a capacitor, a switch, and a load resistor. During the measurement of a spectrum, the switch is open, and the electron charge generated in the photodiode is stored in the capacitor. The longer time we keep the switch open, the more charge we build. Once we have built a strong charge level, the switch is closed, and the stored electrons can flow in the circuit as a current we can measure.

As already mentioned, the detector has a maximum charge that can be stored – called the saturation charge. The integration time can therefore be used as a parameter to control the signal level. In general, we want a signal level that is 80 – 90 % of the saturation level. It is, however, not always practical to integrate for a long time. One example would be if the measurement time is limited by external factors – like the sample passing by the spectrometer at high speed for instance. Another limiting factor is the dark noise of the detector which also rises with integration time.

Any detector generates random charges over time. If the signal is very weak and you integrate for a long time, this dark level might saturate the detector before you even start to see any signal level. See Figure 18 for an example of dark level as a function of integration time for a typical detector at room temperature. As can be seen, below 100 milliseconds (10-1 s) the dark level is low and almost independent of the integration time. However, for an integration time of 10 seconds, the detector is almost completely saturated by dark signal alone and therefore we cannot measure any signal. This means that at room temperature we have to keep the integration time below a few hundred milliseconds.

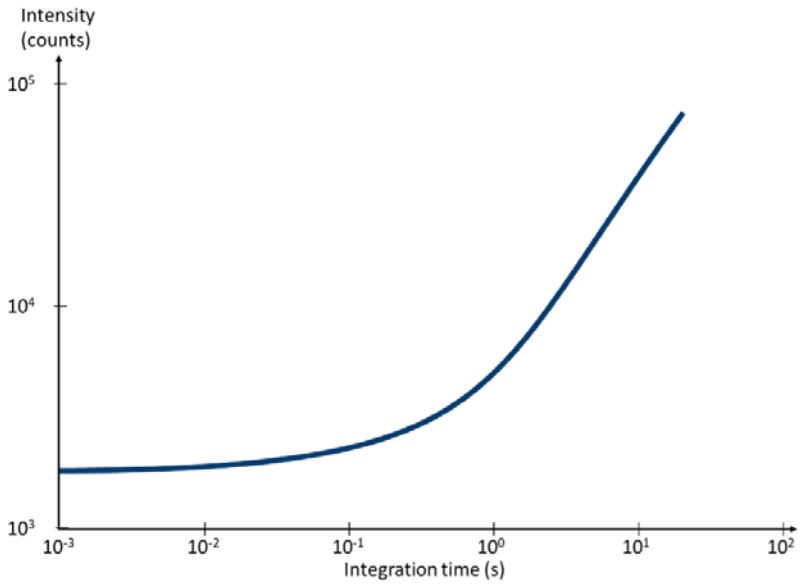



Figure 18: Dark level as a function of integration time for a CCD detector.

The way to counteract the dark level is to decrease the temperature. In Figure 19 the dark level versus integration time is shown for the same detector as in Figure 18. From Figure 19 we can see, that lowering the chip temperature to -10 degrees C will enable us to integrate for around 10 seconds before the dark level starts to rise. This means we can increase our integration time by a factor of 100 and thereby measure a 100 times weaker signal than at room temperature.

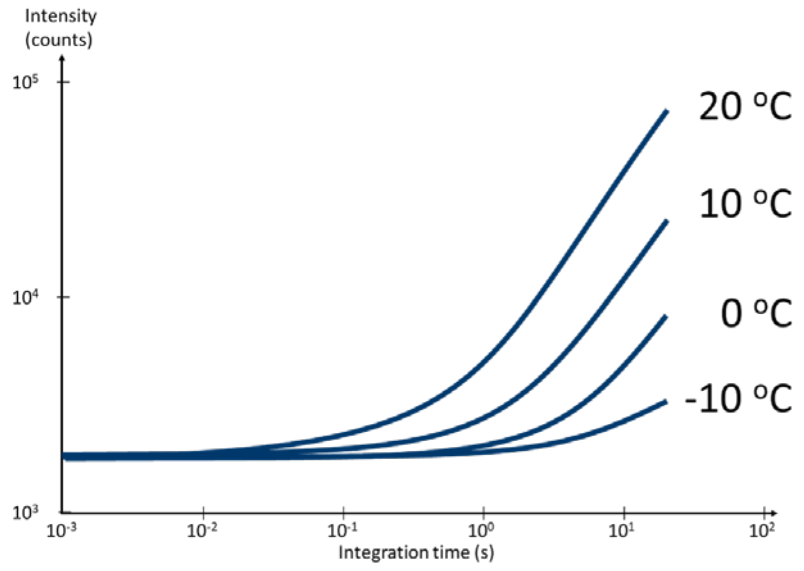



Figure 19: Dark level as a function of integration time at four different chip temperatures.

## High sensitivity detector

- Choose a detector with high QE in your wavelength range
- Choose a detector with a small well depth (but be aware of noise)
- Use a long integration time and cool the detector

## Signal-to-noise level

The generation of charge in the diode array detector is a statistical process. This means that even if we repeat the same measurement say 10 times with the exact same optical signal input we will get 10 slightly different readings (counts). The average (mean) level of our readings is the signal level and the variation around the average is the noise. The noise is often characterized either by the standard deviation or the peak-to-peak difference

The signal-to-noise ratio (SNR) is defined as the average signal level over the number of measurements divided by the standard deviation over the same number of measurements as shown on Figure 20.

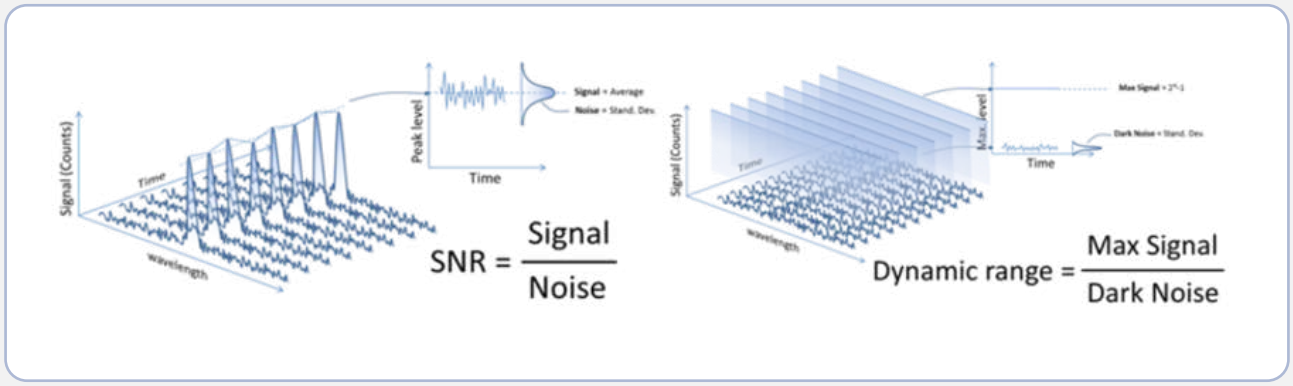



Figure 20: Definitions of SNR and dynamic range.

The SNR determines how small variations in the signal level you can measure. Therefore, SNR is mostly relevant when you have medium to strong signals.

In contrast, the dynamic range determines the largest possible difference in signal level that you can measure. The dynamic range is defined as the maximum possible signal level (detector saturation) divided by the dark noise. The dark noise is the standard deviation of the detector reading in the absence of optical input.

The dark level and the dark noise are often confused but they are not the same. The dark level is the signal level in case of no optical input whereas the dark noise is fluctuation around the dark level. The dark level is often several 1,000 counts whereas the dark noise is often 10 – 30 counts.

If your typical signal level is relatively strong and you need to measure small variations in the signal level you need a spectrometer with a high SNR.

If your typical signal level varies several orders of magnitude you will need a spectrometer with a high dynamic range.

If your signal levels are very weak you will need a spectrometer with high sensitivity as described in the previous section.

A high SNR and dynamic range go hand-in-hand and are generally obtained by choosing a detector with a large electron well. As described earlier on, for a large electron well the relative influence of a single randomly generated electron is very little. Detectors with large electron wells are typically NMOS or CMOS type detectors.

It is important to note that detectors with large electron wells require a lot of photons to fill up and hence they will appear to have low sensitivity, but a high signal-to-noise ratio as described in the section about pixel well depth on page 24.

**High SNR and dynamic range**

- ✔ Choose a detector with a large electron well

## Stability

Spectrometers used to be laboratory instruments operated by skilled personnel in controlled environments. Nowadays, however, spectrometers are used by non-skilled persons in both indoor and outdoor environments exposing the instruments to huge variations in temperature, vibration, shock, and humidity. For this reason, the spectrometer must be designed to operate within the specified performance under these external influences.

The external influences can cause the position of the optical elements inside the spectrometer to shift from their nominal position which in turn causes the spectrometer to go out of wavelength calibration and/or deteriorate the resolution.

In general, reflective optical elements – like mirrors and reflection gratings – are more sensitive to external influences than transmissive elements. We will illustrate this by a simple example with a mirror versus a window – i.e. a flat optical element. Figure 21 a) shows the well-known reflection on a flat mirror surface. When the mirror is rotated by an angle Θ, the reflected light is rotated by two times Θ as shown in Figure 21 b. The transmission through a flat window is shown in Figure 21 c) but, when the window is rotated by Θ the transmitted light is not rotated as shown in Figure 21 d). The rotation of the window will lead to a small displacement of the transmitted beam but, for relatively thin windows this displacement is negligible. This fundamental difference between reflective surfaces and transmissive surfaces means that transmission optics are almost insensitive to any external influence that could cause a rotation of the optics. Such external influences could be vibrations or mechanical stresses due to differences in the thermal expansion coefficient of the glass and the metal mounts

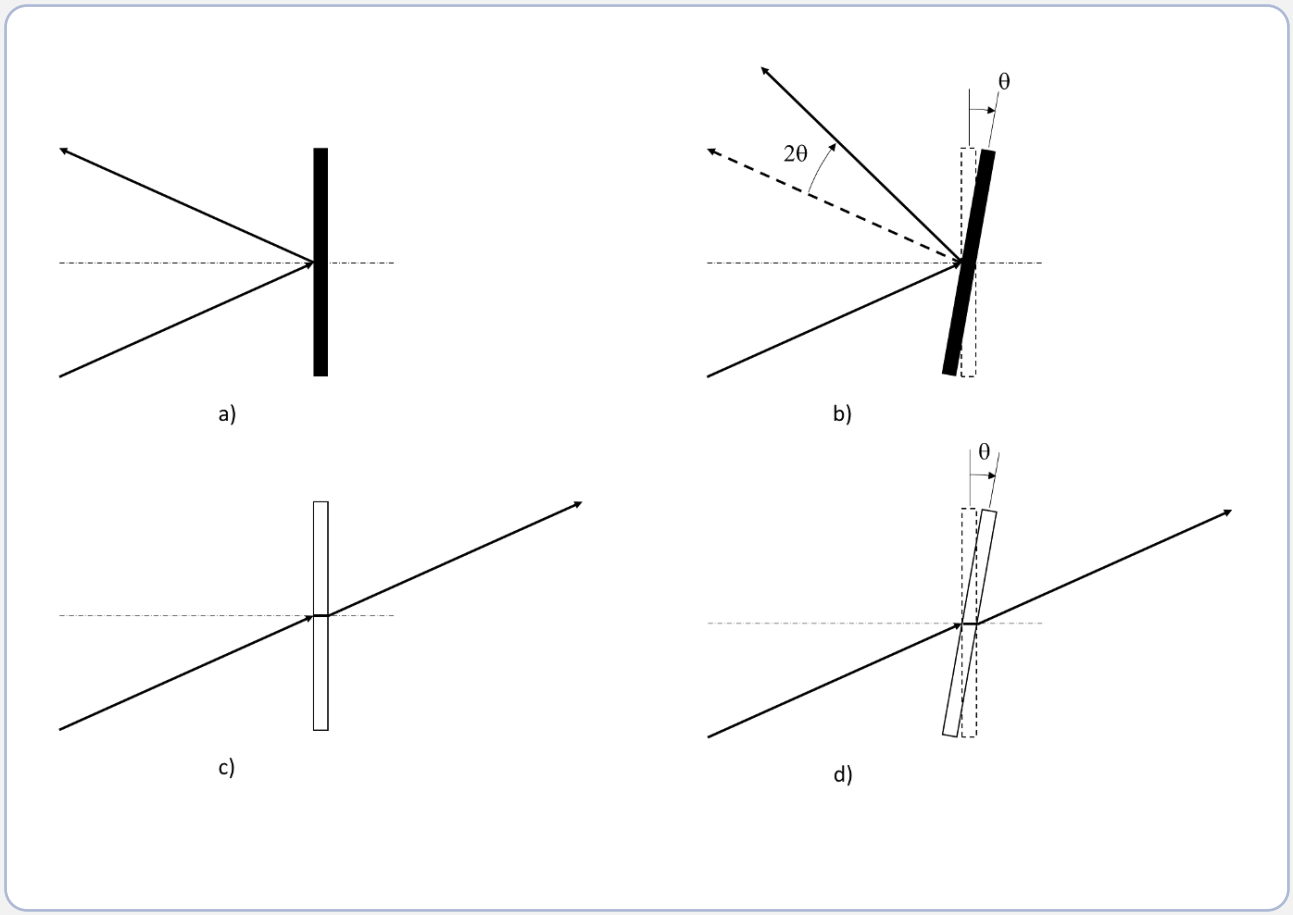
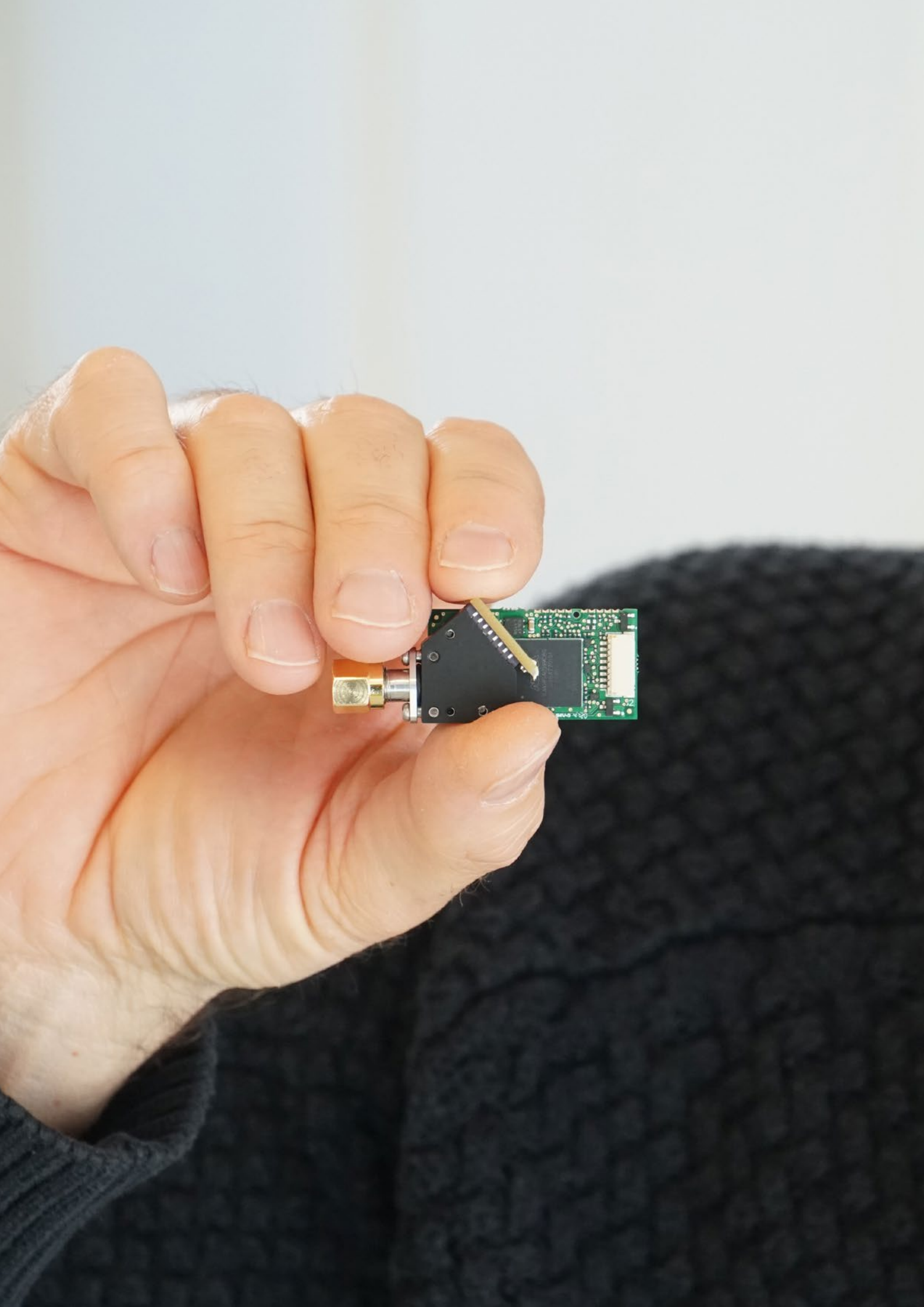



Figure 21: Illustration of how reflection and transmission of a mirror and through a window are influenced by the rotation of the element. a) reflection in a mirror b) reflection angle shifts by 2 times the rotation angle of the mirror c) transmission through a window d) the transmission angle through the window does not change with rotation.

## Stability

- ✔ Choose lenses and transmission gratings for high stability against temperature and vibration



# Coupling into your spectrometer

Any optical spectroscopy system must collect light scattered, transmitted through, or reflected from a sample. The design of the collecting optics is a very important part of your system design. If the collecting optics is not well designed, you can lose a lot of light.

## General considerations

As described in the Section about the sensitivity of the spectrometer, the maximum light that can be collected by an optical system is given by the Etendue:

$$Maximum\ Etendue = Area_{\square} NA_{\square}^2 = Area_{\square} \sin^2(\theta_{\square})$$

The maximum amount of light that the spectrometer can collect is thus given by the slit opening area times the numerical aperture (NA) of the spectrometer squared:

$$Maximum\ light\ collected\ by\ spectrometer = Area_{slit} NA_{spectrometer}^2 = Area_{slit} \sin^2(\theta_{spectrometer})$$

Likewise, the maximum amount of light that is emitted from the sample is given by the area of the sample, and the solid angle that the sample is emitting light within.

$$Maximum\ light\ emitted\ from\ sample = Area_{sample} NA_{sample}^2 = Area_{sample} \sin^2(\theta_{sample})$$

The purpose of the collection optics is to match the spectrometer Etendue with the sample Etendue but, this is not always possible. Let us consider some examples to illustrate how it works.

## Example 1: Sample Area > slit area, sample NA < spectrometer NA

If the sample is larger than the slit area of the spectrometer and the NA of the sample is smaller than the spectrometer, we have a good chance of collecting most of the light from the sample as sketched in Figure 22. All of the light in the green area will be coupled into the spectrometer.

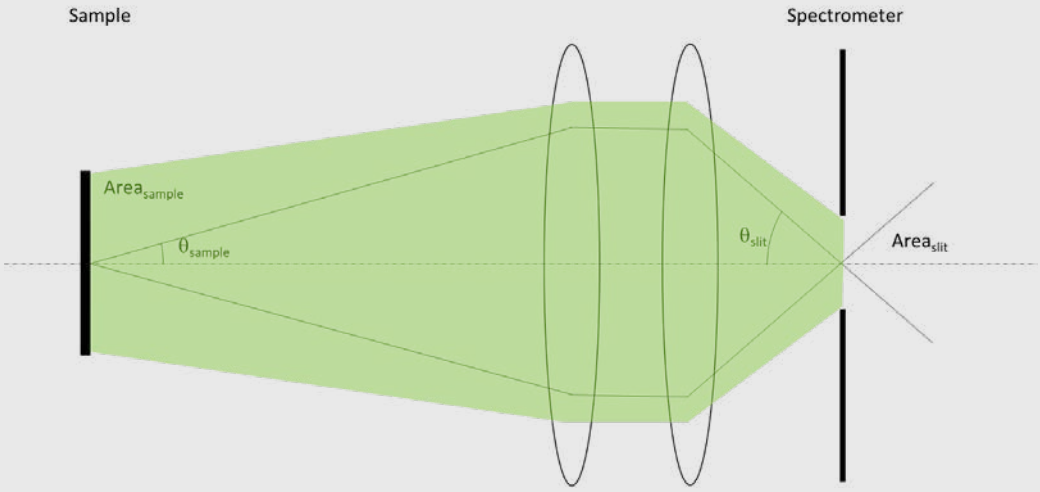



Figure 22: Coupling light from a large sample area emitting in a small NA

## Example 2: Sample area > slit area, Sample NA > spectrometer NA

In the case where both the sample area and sample NA are larger than the spectrometer's slit area and NA we will never be able to collect all the light emitted by the sample as sketched in Figure 23. The light in the red areas is blocked by the slit whereas the light in the green area is coupled into the spectrometer.

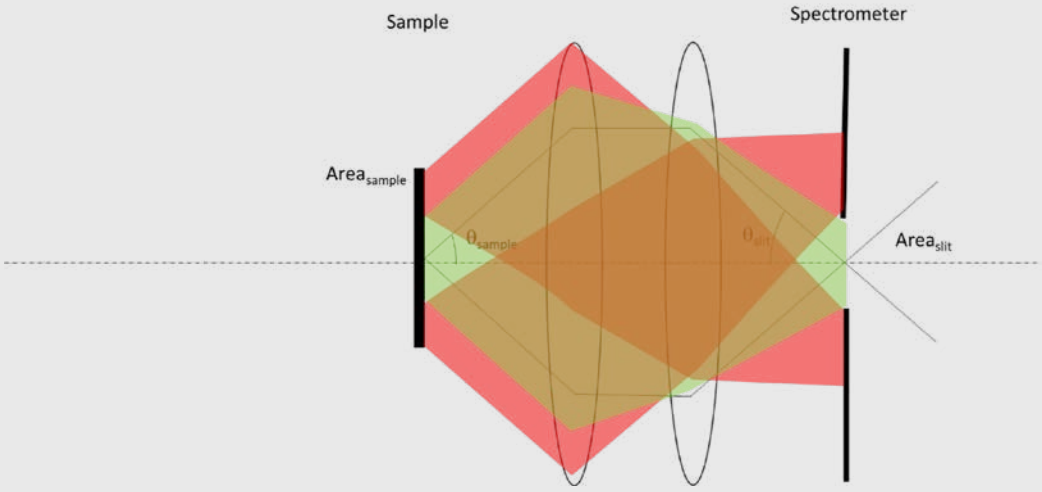



Figure 23: Coupling from a large sample area and large sample NA.

There are two basic ways by which you can design your collection optics: with fiber optics or with free space optics.

## Fiber optics

The general benefit of fiber optics is the ease of use and alignment. Basically, you can point one fiber-end towards your sample and the other fiber end towards the slit of the spectrometer. The fiber will guide the collected light from the sample towards the spectrometer. Because the guide is somewhat flexible you can even bend the fiber or have the spectrometer location move relative to the sample.

Figure 24:Illustration of coupling into the spectrometer using fiber optics.

Fibers used for spectroscopy are mostly multi-mode fibers. These have typically core diameters ranging from 50 microns to 1000 microns and numerical apertures from 0.1 to 0.5. As discussed previously the core area and NA must be chosen to match the slit area and NA of the spectrometer.

The drawback of using fibers is mostly that you lose up to 50% of the light by coupling in and out of the fiber. Furthermore, the fiber core is round whereas the slit used for spectroscopy is mostly rectangular leading to a poor area match as sketched below. The green area is the slit opening which will collect light from the fiber core. The read area, however, is the part of the fiber core that is blocked.

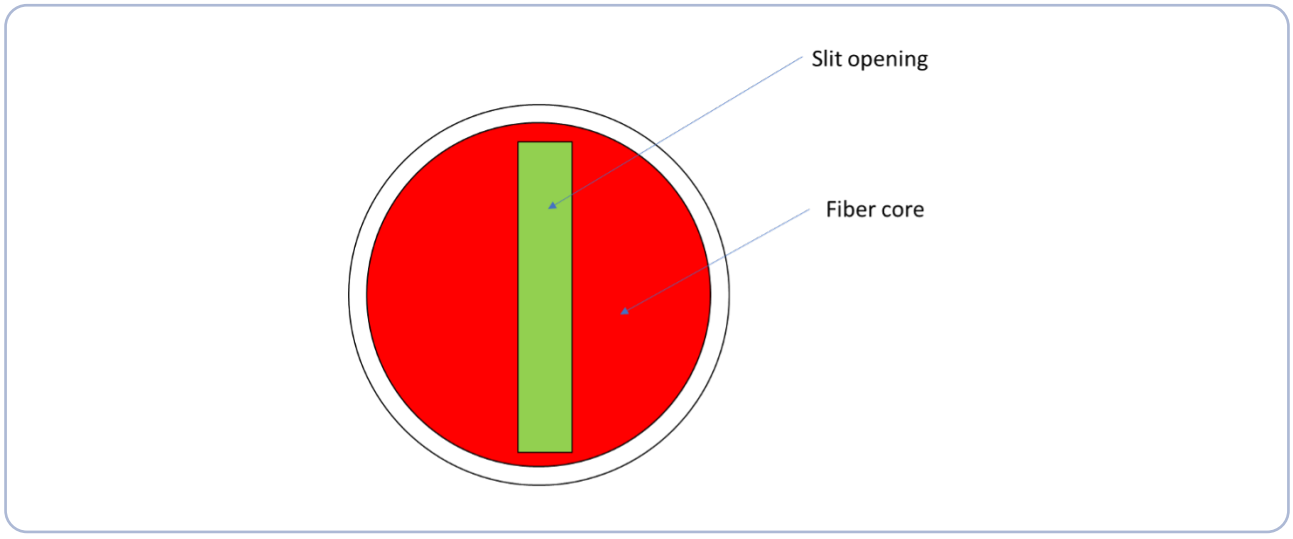



Figure 25: Slit opening (green area) and fiber core (red area).

The multimode nature of the optical fiber can also cause some unwanted phenomena. First of all, when you couple from your sample and into the fiber, you have to make sure to fill the fiber core evenly – both across the area and across the numerical aperture. For in-homogenous samples, this might be hard to obtain and therefore, it can be beneficial to use a so-called diffuser between the sample and the fiber end. A diffuser however is also attenuating your signal significantly.

Multimode fibers are also very sensitive to temperature, pressure, and bending. The way this typically shows up in spectroscopy is as a small unstable intensity ripple on the spectrum that changes/fluctuates with temperature, pressure, and movement of the fiber.

One way to accommodate the mismatch between the round fiber core and the rectangular slit is to use a bundle of fibers arranged in a line-to-round configuration. Towards the sample, the bundle of fibers is arranged in a disc shape and towards the slit, the fibers are arranged in a line as shown below. In case you do not have a fiber bundle it is always better to use a fiber filling out the entire slit height as illustrated in Figure 25 since the amount of input light will be higher.

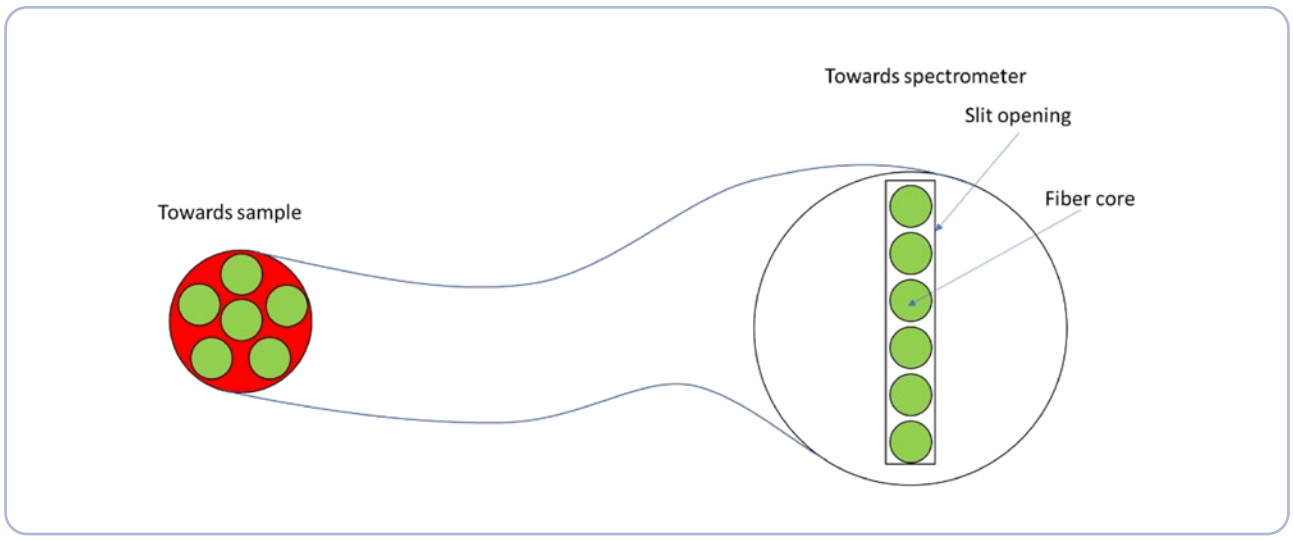



Figure 26: Fiber bundle in round-to-line configuration.

Finally, it is important to choose the right fiber for the wavelength range you are using it for. Especially, in the UV region, you need to use so-called solarization resistant fibers. Normal fibers will slowly degrade and become more and more lossy as they get exposed to UV light. In the NIR region, it is important to use low-OH fibers since OH has a strong absorption overtone at 1400 nm.

## Free space optics

Figure 27:Illustration of coupling into the spectrometer using free space optics.

Free space optics means that the collection optics are built using classical optical elements like lenses and mirrors. The major benefit of free space optics is that the loss can be very low. Good lenses with AR-coatings can provide 98-99 % transmissivity for instance.

The main drawback of free space optics is that the alignment is more difficult than with fibers. All the different optical elements need to be held in place and in the right (focal) positions even during temperature changes or vibration which is not a trivial task.

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