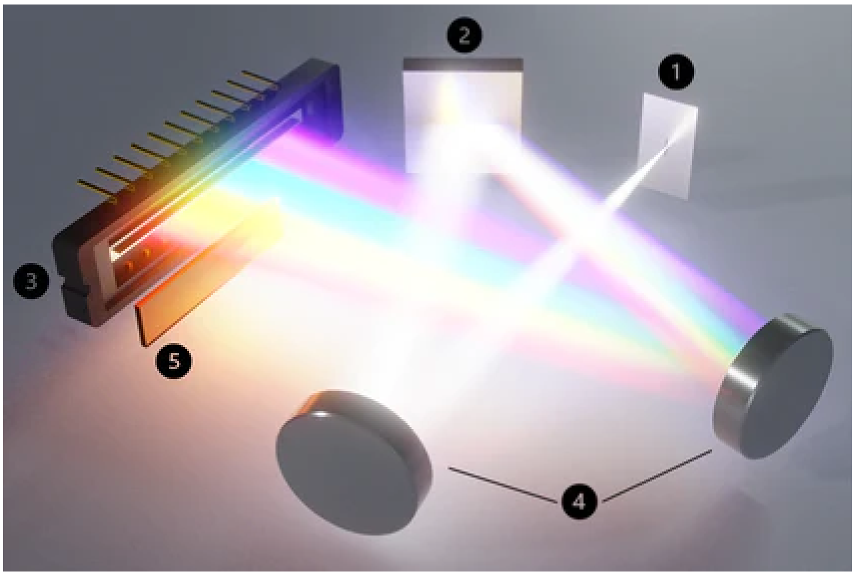
How Does a Spectrometer Work? Principles & Optics



A spectrometer consists of (1) an entrance slit, (2) a diffraction grating or prism, (3) a detector, (4) routing optics, and (5) higher order filters.

Optical spectrometers (https://www.ossila.com/en-eu/collections/spectroscopy) are the most common **type of spectrometer (https://www.ossila.com/en-eu/pages/spectrometer-application-notes)**. They take light, separate it by wavelength and create a spectra which shows the relative intensity of these separate wavelengths. This basic principle has a wide range of **applications and uses (https://www.ossila.com/en-eu/pages/spectrometer-application-notes)**.

Broadly speaking, all optical spectrometers consist of an entrance slit, a diffraction grating or prism, a detector, and routing optics. The entrance slit allows light into the spectrometer, where a system of mirrors or lenses routes it first onto a diffraction grating or prism, and then onto the detector. The grating or prism splits the light into its constituent wavelength components, and the detector records the light intensity as a function of wavelength. If the spectrometer has a large spectral range, it may also have filters to stop higher order light from reaching the sensor. Most **optical spectrometers (https://www.ossila.com/en-eu/products/optical-spectrometer?variant=42326523379928)** operate over the UV, visible, and infrared (or near-infrared) regions of the electromagnetic spectrum.

Spectrometers can be designed and built using a number of different optical configurations. These include the **Littrow configuration (https://www.ossila.com/en-eu/pages/spectrometer-working-principles#littrow-configuration)**, the **Ebert-Fastie configuration (https://www.ossila.com/en-eu/pages/spectrometer-working-principles#ebert-fastie-configuration)**, the **Czerny-Turner configuration (https://www.ossila.com/en-eu/pages/spectrometer-working-principles#czerny-turner-configuration)**, and the **concave aberration-corrected holographic grating configuration (https://www.ossila.com/en-eu/pages/spectrometer-working-principles#concave-holographic-configuration)**. Careful choice of components and configuration can avoid aberrations, which result in distorted or blurred spectra.

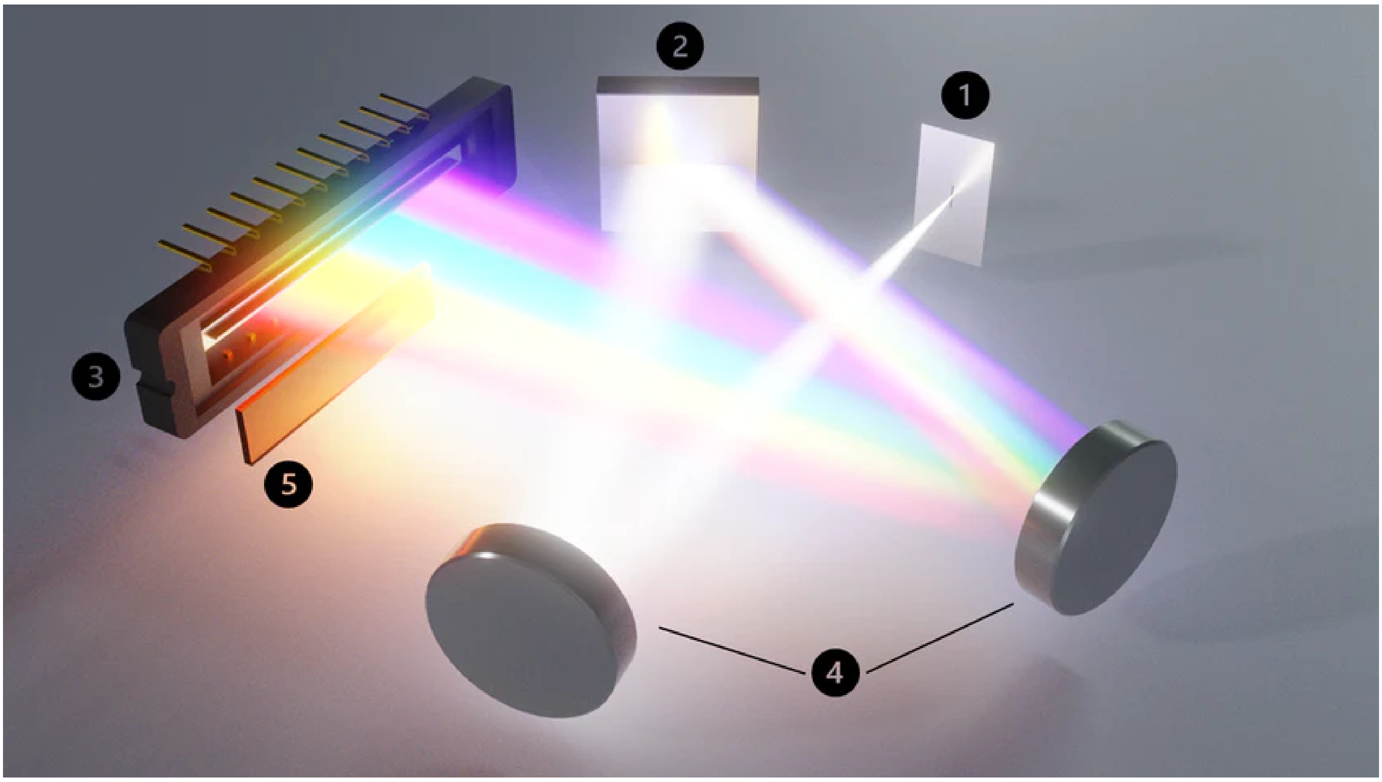
For more information on types and uses of spectrometer, see **What is a Spectrometer? Types and Uses (https://www.ossila.com/en-eu/pages/spectrometer-application-notes)**

Contents

- Spectrometer components
    - Spectrometer entrance slit
    - Diffraction grating or prism
    - Spectrometer detector
    - Routing optics
    - Higher order filters
- Spectrometer optics
    - Littrow configuration
    - Ebert-Fastie configuration
    - Czerny-Turner configuration
    - Concave aberration-corrected holographic grating configuration
    - Spectrometer aberrations
- Light Sources for Spectroscopy
    - Monochromatic light sources
        - Light emitting diodes (LEDs)
        - Lasers
    - Broadband light sources
        - Broadband LEDs
        - Tungsten halogen
        - Gas discharge/arc lamps

Spectrometer Components

Return to the top



Optical spectrometer components: entrance slit (1), diffraction grating or prism (2), a detector (3), routing optics (4), higher order filters (5)

Entrance Slit

Light enters the **optical spectrometer (https://www.ossila.com/en-eu/products/optical-spectrometer)** via the entrance slit. Similarly to how the aperture size of a camera affects the brightness and resolution of its photos, the width of the spectrometer entrance slit determines both its ability to measure in low-light conditions and the maximum spectral resolution that you can achieve.

These two characteristics must be balanced against each other as one will always come at the expense of the other. A wide entrance slit allows a lot of light to enter the spectrometer, which allows fainter sources to be measured but reduces the spectral resolution of the system. Conversely, a narrow entrance slit can increase the spectral resolution, but at the cost of signal intensity.

Larger optical spectrometers may have a controllable slit width, while more compact devices like the **Ossila Optical Spectrometer (https://www.ossila.com/en-eu/products/optical-spectrometer)** (which has an entrance slit width of 25 µm) usually have a fixed width.

Diffraction Grating or Prism

The optical diffraction grating is the component that splits the light into its constituent wavelength components. There are a number of different types of gratings including transmissive, reflective, ruled, and holographic. Each has their own advantages and disadvantages when compared to one another, and there is no one superior design.

The design of the grating determines to what degree the light is spread out. Much like the slit, there is a trade-off between resolution, range, and signal strength.

Diffraction gratings can be described by the equation:

$$d(sin\theta_m - sin\theta_i) = m\lambda$$

Return to the top

Where d is the grating spacing, θ_m is the diffraction angle of the m^{th} diffraction order, θ_i is the angle of incidence, and λ is the wavelength of the light. From this, you can see that decreasing the grating spacing will increase the angular range of diffraction. Therefore, a smaller range of wavelengths will reach the detector with reduced signal strength, but with higher resolution. Conversely, increasing the grating spacing gives a bigger range of wavelengths but with lower resolution.

The grating spacing is usually quoted in terms of groove density, which is equal to $1/d$ and is given in units of grooves mm^{-1}.

In some spectrometers, the diffraction grating can be rotated to allow different wavelengths to hit the detector. Here, the acquisition window will be selected according to need. Similarly, some spectrometers have multiple gratings with different groove densities, which can be selected between.

Some designs of optical spectrometer use a prism as the dispersive element in place of a diffraction grating, but due to the higher cost of prisms and the lower resolution images that they give, this is not common.

Detector

The optical detector records the intensity of the light that reaches it as a function of its wavelength. Spectrometer detectors consist of a row of light sensitive pixels, each of which corresponds to a particular wavelength. Each pixel will generate an electrical signal of intensity proportional to how much light is falls on it.

Charged-coupled devices (CCDs) are the detector of choice for spectrometers due to their high dynamic range and uniform pixel response. To reduce unwanted noise in the spectra, CCDs are usually cooled to combat dark current signals.

Routing Optics

Internal routing optics direct the light from the entrance slit onto the diffraction grating or prism, and then onto the detector.

Curved mirrors are generally preferred over lenses as they introduce fewer image aberrations. There are many possible configurations for the optics (e.g. Fastie-Ebert, Czerny-Turner) which each have relative advantages and disadvantages regarding optical aberrations, stray light, and size.

Higher Order Filters

If the wavelength detection range of an optical spectrometer spans more than one diffraction order, a filter may be necessary to partially cover the detector and block higher order light from reaching the sensor.

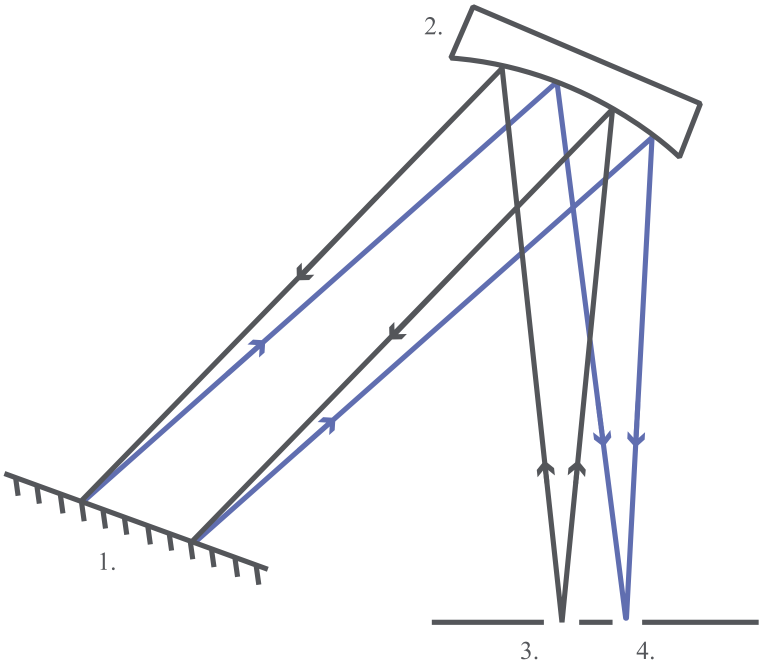
Spectrometer Optics

Return to the top

Littrow Configuration

The Littrow configuration is the simplest design utilising a plane reflection grating. Although it is not commonly found in spectrometers today, it is still used to characterise diffraction gratings (see '**Grating blaze wavelength (https://www.ossila.com/en-eu/pages/spectrometer-application-notes#grating-blaze-wavelength)**').

This configuration consists simply of a spherical mirror and a plane grating. The light enters the spectrometer through an entrance slit and is collimated by the mirror. The reflected light is then incident on the diffraction grating, as is shown below. The diffraction order of interest is directed back towards the mirror, where it is reflected towards the exit slit, which is spatially very close to the entrance slit.



Schematic of the Littrow configuration showing 1.diffraction grating 2.spherical mirror 3. entrance slit and 4. exit slit

Although this configuration has a very high wavelength resolution, the risk of stray light, internal reflections and multiple dispersions is significant.

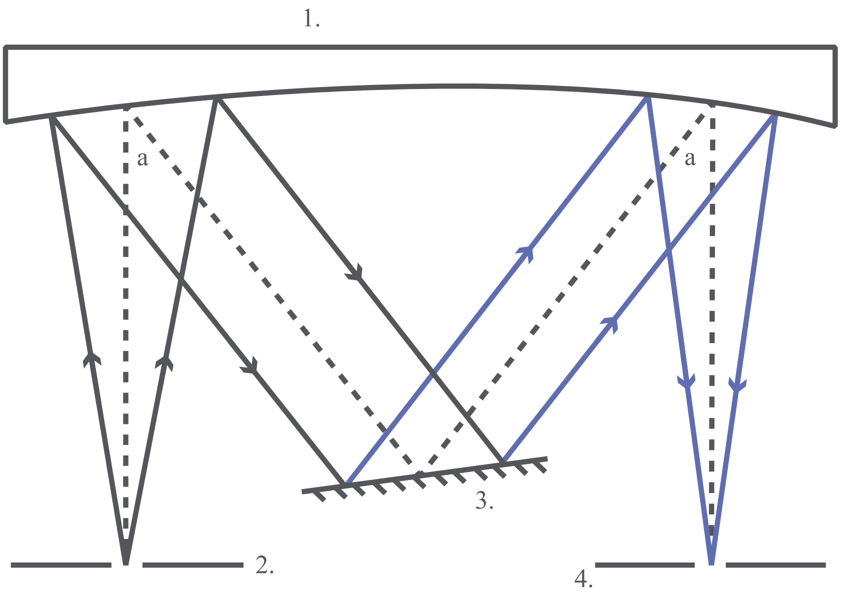
Ebert-Fastie Configuration

The Ebert spectrograph was first described by Hermann Ebert in 1889. After many decades of relative obscurity, the design was resurrected by William G. Fastie in 1952, who included curved slits to remove astigmatism (see 'Aberrations present in spectrometers') and reduce wavelength errors at the exit slit [1].

The Ebert-Fastie (sometimes referred to as Fastie-Ebert) configuration is composed of a large spherical mirror and a single plane diffraction grating. The light enters the spectrometer through the circularly curved entrance slit and is incident on one portion of the mirror, as illustrated below. The mirror directs the now-collimated light onto the plane grating and the diffracted light is then reflected from a second, separate portion of the mirror. The light reflected from the mirror is then focused through the circularly curved exit slit, after which point it is collected by the detector. Here, the angle between the incident and reflected rays, a, is the same for both reflections from the mirror [2].

Limitations of the Ebert-Fastie configuration include the risk of light being reflected directly from the mirror towards the exit slit without being diffracted and of multiple diffractions.

Return to the top



Schematic of the Ebert-Fastie configuration showing 1.large spherical mirror 2.entrance slit 3.diffraction grating and 4. exit slit

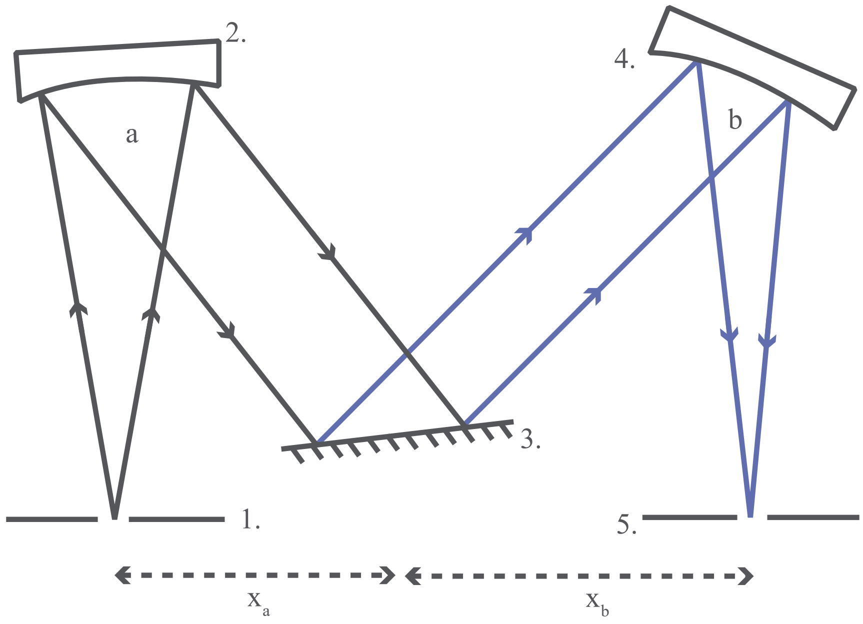
Czerny-Turner configuration

Quite similar in design to the Ebert-Fastie configuration, the most common design used in spectrometers today is the Czerny-Turner configuration. First described in 1930 by M. Czerny and A.F. Turner, the design has since been altered to remove and reduce certain aberrations and has several advantages over the Ebert-Fastie configuration [2].

Instead of a single large spherical mirror, the Czerny-Turner configuration uses two smaller spherical mirrors, as depicted below. Here, the light enters the spectrometer through the entrance slit and is reflected from the first spherical mirror onto a plane diffraction grating. The dispersed light is then reflected by the second mirror and is collected by the detector on the other side of the exit slit.

In Czerny-Turner configurations, the mirrors don't have to be the same size, or placed the same distance from the slits or the diffraction grating. They can even have different radii of curvature. In addition, the reflection angles for the two mirrors, a and b, do not have to be equal and the grating can even be "off-axis", i.e. the distances xa and xb can be different [3].

Return to the top



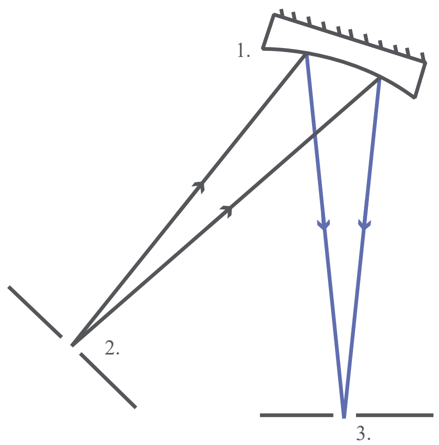
Schematic of the Czerny-Turner configuration showing 1. entrance slit 2.1st spherical mirror 3. diffraction grating 4.2nd spherical mirror and 5. exit slit

This configuration does not allow light to be directly reflected from the entrance to the exit slits, which reduces unwanted reflections and multiple dispersions compared to the Ebert-Fastie configuration. The asymmetrical design allows for better coma correction and a flattened spectral field compared to the symmetrical version (see **aberrations**).

It is possible to fabricate holographic gratings to include physical aberrations that cancel out all optical aberrations at a particular wavelength and drastically reduce them for a large range of wavelengths [4].

Concave aberration-corrected holographic grating configuration

Instead of a plane grating, it is also possible to fabricate concave holographic gratings that correct for optical aberrations. In this case, the diffraction grating is the only optic needed: the light enters the spectrometer through the entrance slit and is diffracted by the grating, which focuses the light onto the exit slit.



Return to the top

Schematic of a concave aberration-corrected holographic grating configuration showing 1. Concave holographic diffraction grating 2. entrance slit and 3. exit slit

As only a grating is needed for this configuration, errors due to multiple reflections, imperfect mirrors, and thermal effects are reduced. A higher signal-to-noise ratio is also possible due to decreased reflection losses. This design is simple to align, inexpensive and compact.

Spectrometer Aberrations

There are several different types of aberration present in spectrometers that can cause images and spectra to be distorted or blurred. It is possible to significantly reduce the effect of these aberrations using specific components and configurations. In general, mirrors (and gratings) are used for collimation instead of lenses as they result in a much lower degree of aberration. However, certain aberrations can still arise.

Spherical aberration

Spherical aberration arises when rays are reflected from a spherical surface; for example, a spherical mirror. When collimated light rays are incident far from the optical axis (the centre) of the mirror, the reflected rays are focused closer to the mirror surface than those that were incident on or near the optical axis. This is illustrated in the figure below (where it should be noted that the different colours are simply for ease of viewing and do not correspond to different wavelengths/colours of light).

Spherical aberration can be avoided by using parabolic mirrors; however, these are more difficult to make and therefore more expensive.

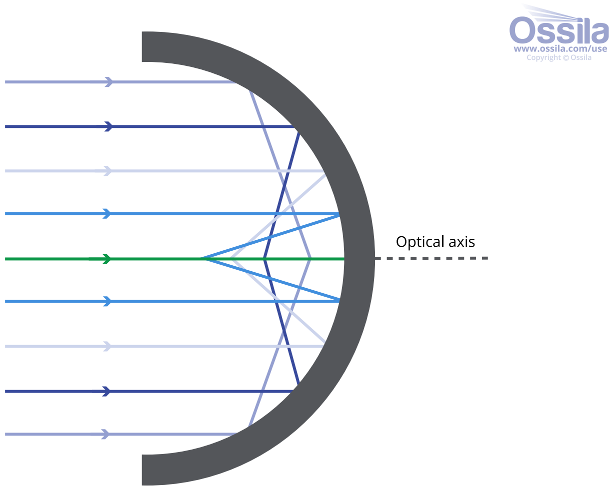


Illustration of parallel rays affected by spherical aberration from a spherical mirror

Coma

Return to the top

A point source - for example, a star - as viewed through a telescope with comatic aberration will appear to have a comet-like tail; hence, the term "coma". This is due to the fact that when parallel rays are incident at an angle to the optical axis of a spherical mirror, the reflected rays do not have a common focus. This is illustrated in the left-hand figure below (where it should be noted that the different colours are for ease of viewing and do not correspond to different wavelengths/colours of the rays) and results in a blurred image. In a spectrum, coma appears as an increased signal on one side of a spectral feature, i.e. an asymmetrical broadening, as illustrated in the right-hand side of the figure below.

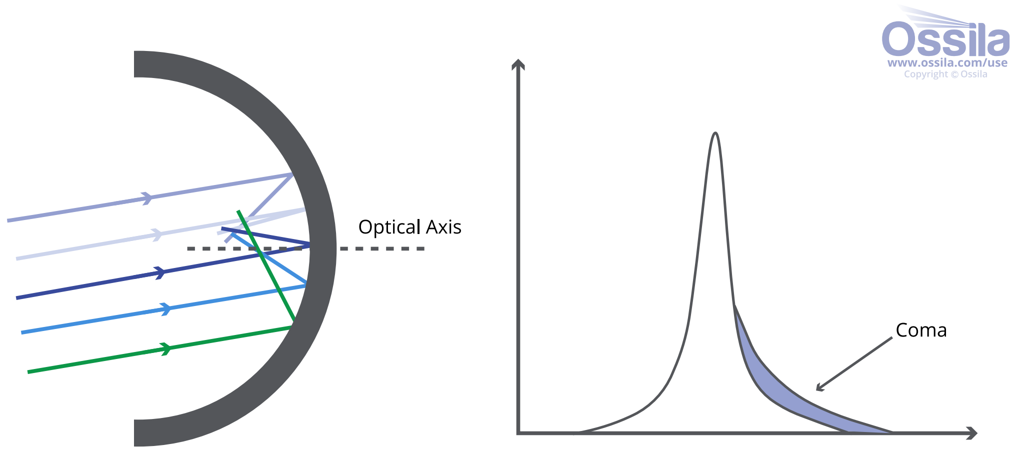


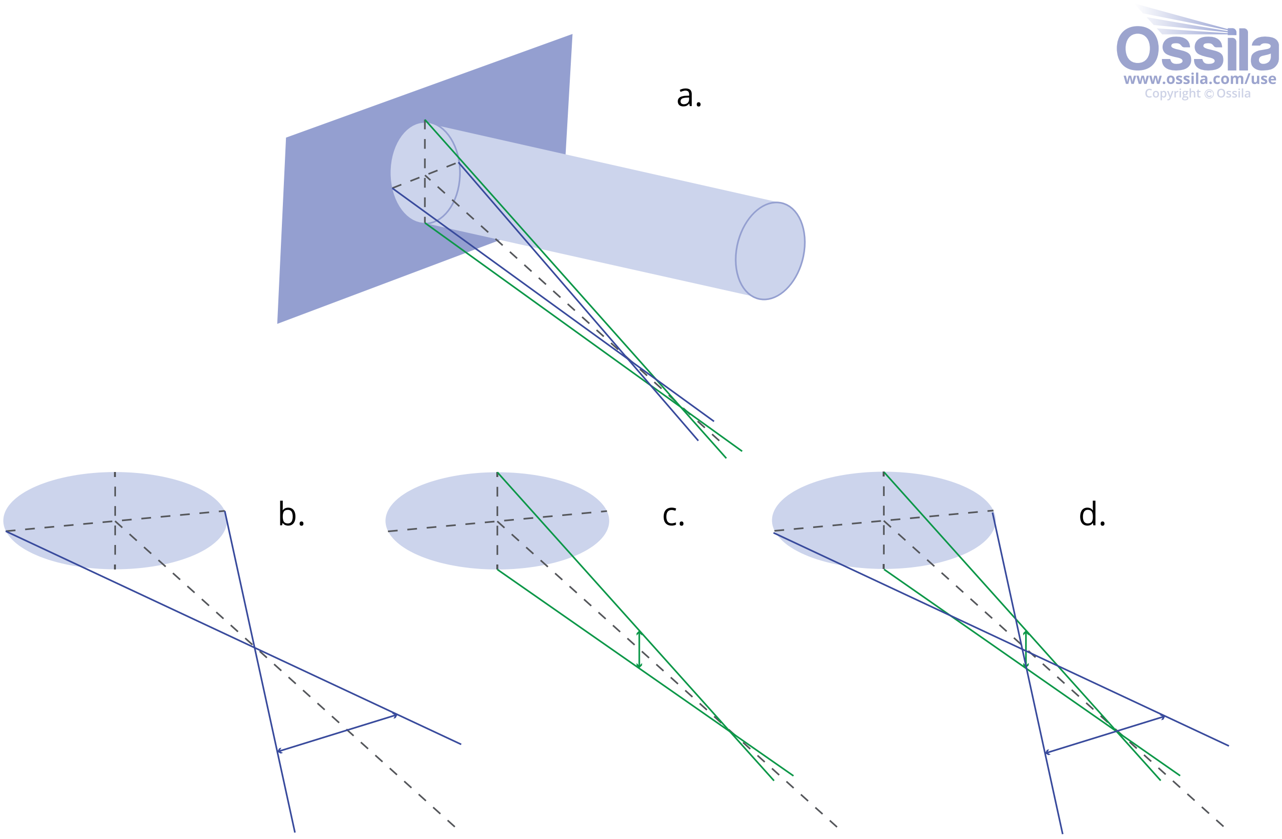
Illustration of parallel rays (left-hand figure) and an example spectrum (right-hand figure) affected by comatic aberration (coma) from a spherical mirror

In Czerny-Turner spectrometers, it is possible to completely eliminate coma at one wavelength, and using a concave aberration-corrected holographic grating configuration, it can be eliminated at a wide range of wavelengths.

Astigmatism

Astigmatism also occurs during the off-axis illumination of a spherical mirror. Here, the rays in the horizontal (transverse) and vertical (sagittal) planes are focused at different points. This is illustrated in the figure below, where it can be seen that the rays in the horizontal plane are focused closer to the mirror than in the vertical plane. This effect results in an elongation of the image and can lead to a loss in spatial resolution and signal-to-noise ratio in a spectrometer.

Return to the top



Effect of astigmatism: (a) Shows an off-axis parallel beam being reflected by a spherical mirror, parts (b) and (c) show the focus in the horizontal plane and the vertical plane respectively, and in (d), it can be seen that these foci occur at different distances from the mirror

Astigmatism can be avoided by using curved slits, as in the Ebert-Fastie configuration, or an aberration-corrected grating [1]. It can also be removed by replacing spherical mirrors with toroidal ones; however, these are still affected by coma and spherical aberration.

Light Sources for Spectroscopy

Monochromatic Light Sources

Light emitting diodes (LEDs)

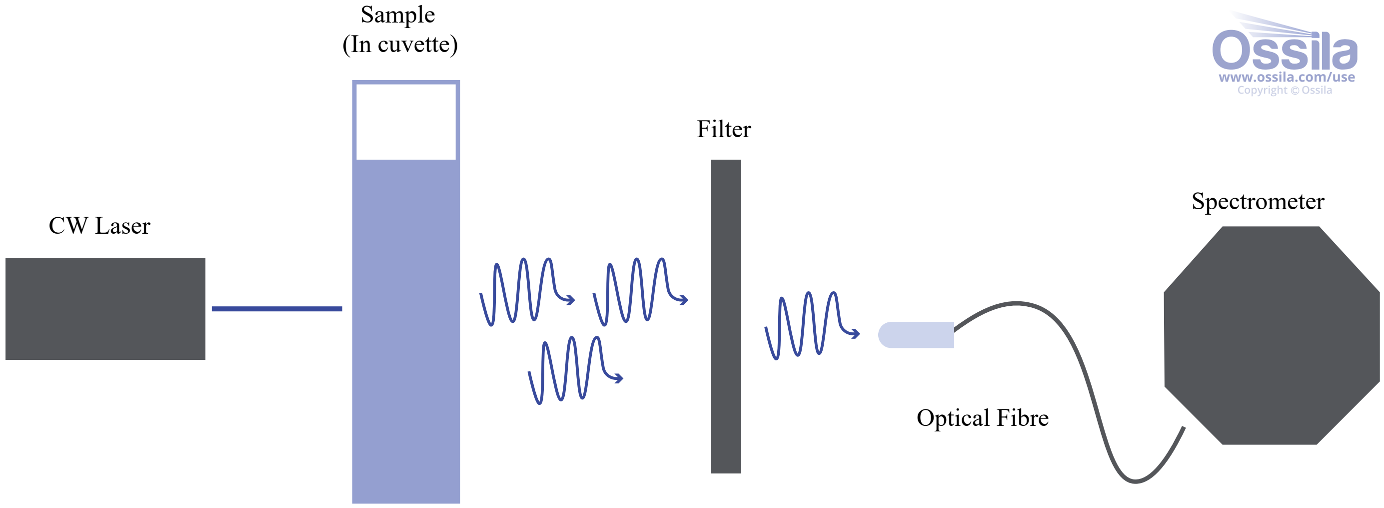
LEDs are a popular monochromatic light source due to their narrow emission spectrum, low power consumption, high stability, long lifetime and fast switching. In the past they were made from inorganic semiconductors, such as gallium arsenide (GaAs) and gallium arsenide phosphide (GaAsP). However, organic LEDs (OLEDs) have now become popular due to the broad range of colours which they are able to produce; by adding different functional groups to organic molecules, it is possible to alter their emission wavelength, making it relatively easy to fabricate LEDs of any colour.

Lasers

Lasers produce monochromatic, coherent, collimated light through the process of stimulated emission (hence LASER, or “**L**ight **A**mplification by **S**timulated **E**mission of **R**adiation”).

There are two types of lasers, continuous wave lasers and pulsed lasers. Continuous wave (CW) lasers produce a constant beam of photons with no fluctuation in power over time. Diode CW lasers are similar in design to LEDs, and are often used for measurements where very high powers are not necessary, such as fluorescence measurements. Compared to continuous wave lasers, diode lasers are much more affordable.

Return to the top



A typical fluorescence setup for spectroscopy, where the sample is illuminated by a monochromatic light source - in this case, a CW laser - and the emitted light is collected by a spectrometer via an optical fiber. The between the sample and the detector blocks light from the excitation source.

Pulsed lasers are very powerful as they are able to deposit very high amounts of energy in a short space of time. The pulse length used for fast spectroscopy is usually on the order of picoseconds (10 - 12 s) or femtoseconds (10 - 15 s), though attosecond (10 - 18 s) pulses are also possible. Pulsed lasers are often used in time-resolved measurements, such as transient absorption (pump-probe), or measurements that require very high energies - for example, as an excitation source for other lasers.

Pulsed lasers can also be used in non-linear optics to produce pulses of different wavelengths, such as in second harmonic generation (frequency doubling) or optical parametric amplification.

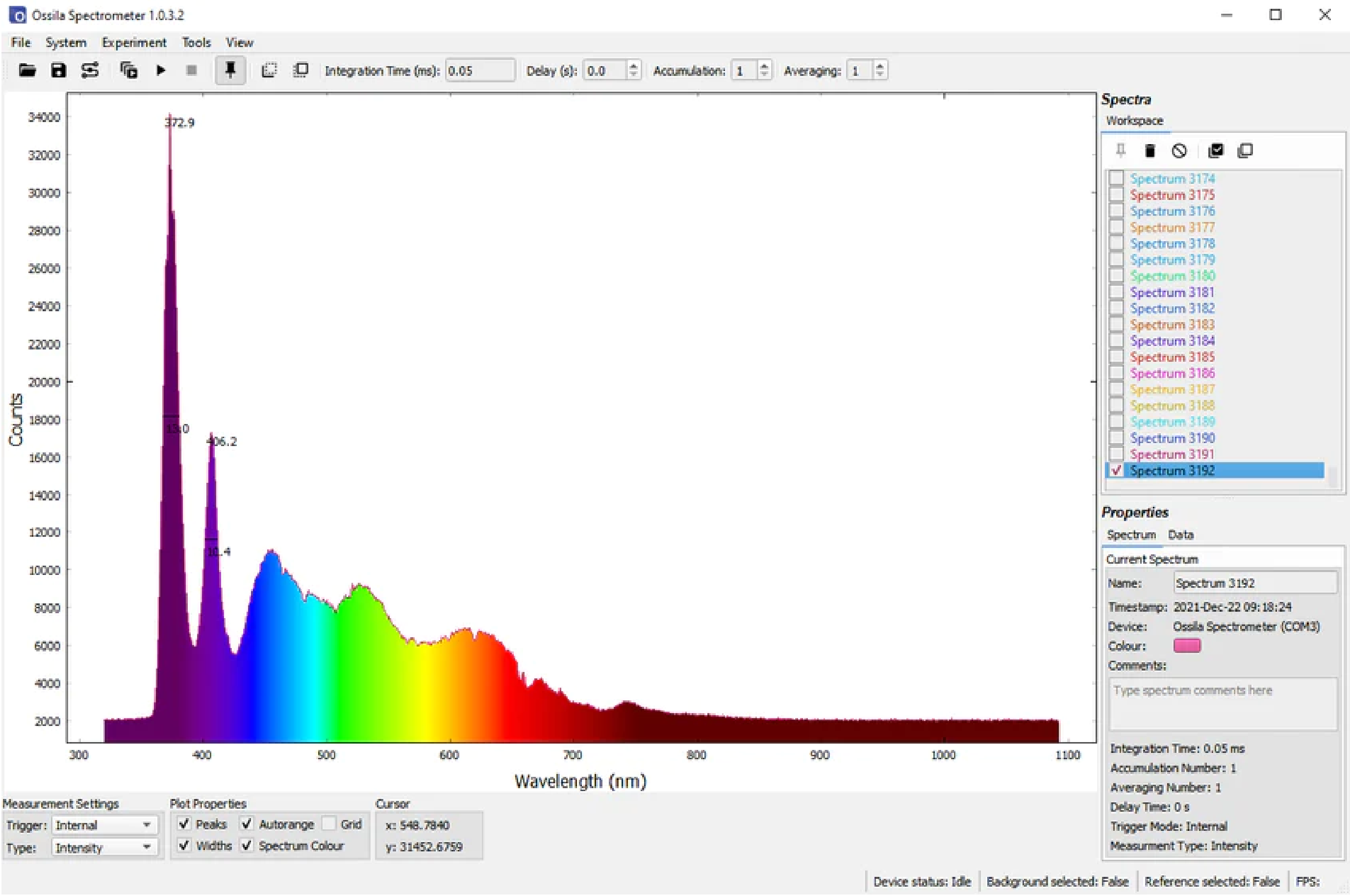
Broadband Light Sources

Broadband LEDs

Although individual LEDs produce light with a very narrow spectrum, multiple LEDs can be combined to produce a broader spectrum. It is also possible to coat the LEDs with phosphors - materials that absorb UV and blue light and re-emit in the visible - in order to cover the entire UV-vis spectrum. In this way, the **Ossila Broadband White Light Source (https://www.ossila.com/en-eu/products/broadband-white-light-source)** is able to produce light covering a spectral range of 360–900 nm.

LED light sources are typically more expensive than incandescent and gas discharge lamps, but their extended lifetimes mean they need to be replaced much less often, making them cheaper in the long run. They are also significantly more efficient as there is no energy lost through heat and their “warm up” and “cool down” times are instantaneous. Broadband LEDs can be powered over USB, are less fragile than lamp type light sources, and do not contain hazardous gases.

Return to the top



Spectrometer software showing the spectrum for the Ossila Broadband White Light Source as recorded by the Ossila Optical Spectrometer (https://www.ossila.com/en-eu/products/optical-spectrometer)

Tungsten halogen

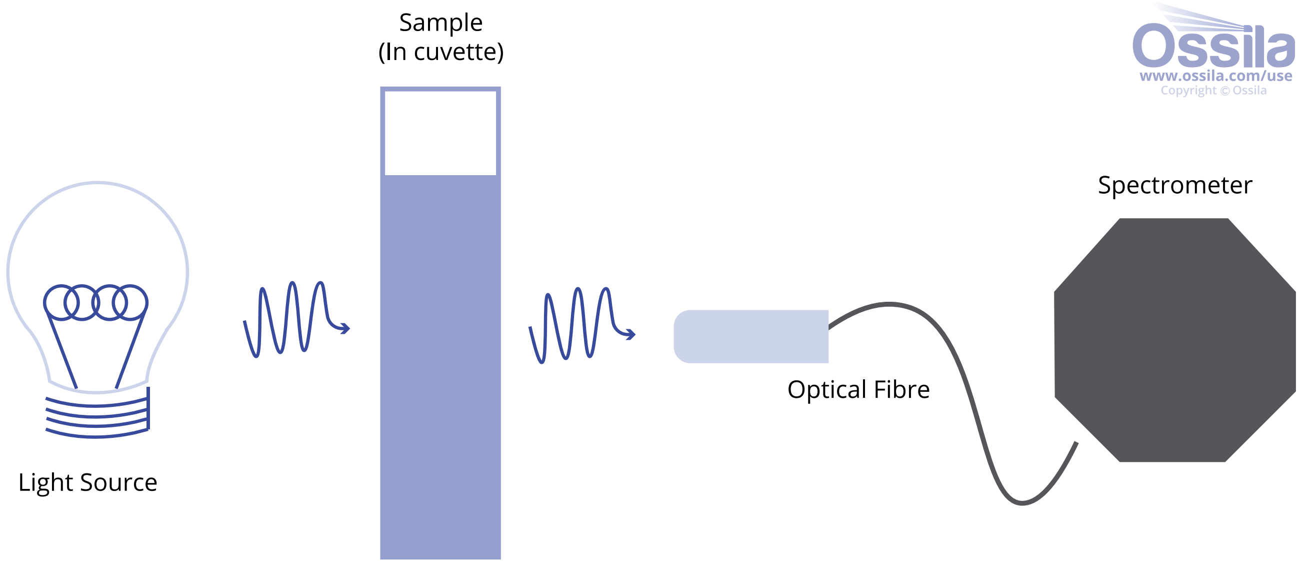
Tungsten halogen lamps (also referred to simply as halogen lamps or as quartz iodine lamps) are a type of incandescent lamp that emit from the UV-visible light boundary to the infra-red region. The exact spectral range depends on the temperature of the filament, but they are generally not suitable for measurements in the UV.

Tungsten halogen lamps consist of a tungsten filament inside a glass bulb. For this, quartz glass is used as it has a high melting point and is capable of withstanding high pressures without breaking. The capsule is filled with a mix of an inert gas, such as krypton or xenon, and a halogen, such as iodine or bromine.

The tungsten filament is heated by passing an electric current through it so that the filament becomes incandescent (it emits light). Most of the energy is emitted in the infrared, making tungsten halogen lamps very inefficient for day-to-day lighting but suitable for spectroscopy measurements in the IR region.

The inert gas in the glass bulb reduces the evaporation and oxidation of the tungsten filament, while the halogen helps to redeposit the tungsten particles back onto the filament through the “halogen cycle”. This increases the lifetime of the filament compared to incandescent lamps that do not contain any halogen, and reduces blackening caused by the deposition of tungsten particles on the inside of the glass.

Return to the top



Typical UV-vis transmission setup, with the sample illuminated by a light source. The transmitted light is collected by a spectrometer via an optical fiber.

Gas discharge/arc lamps

Arc lamps are a type of gas discharge lamp which produce light by sending an electric discharge current through a plasma (an ionised gas). Generally, an electric field is applied between two electrodes inside a heat-resistant glass tube filled with the gas. The atoms become excited through ionisation or through collisions with electrons or other gas atoms or ions. When the atoms or ions relax back to the ground state, a photon is emitted. The wavelength of this photon is characterised by the gas used.

Deuterium arc lamps are commonly used in UV spectroscopy as they produce a continuous spectrum from around 180-370 nm (though there is non-continuous emission up to 900 nm). They are almost always combined with a tungsten halogen lamp to allow measurements in the UV, visible, and NIR.

Xenon arc lamps typically produce a continuous spectrum over a wavelength range of 190-1100 nm. This makes them more efficient than deuterium/tungsten halogen lamps as they can cover the same spectral range with only one lamp. However, they are both more expensive and less stable.

Light from discharge gas lamps is unpolarised and incoherent. Often they take a while to reach full light output power, but despite this, they are still more efficient than incandescent lamps.

Back to Top

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Return to the top

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Return to the top

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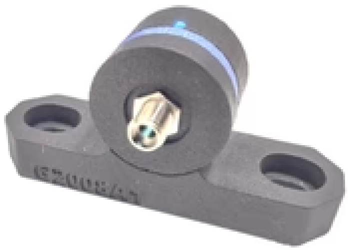

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Return to the top

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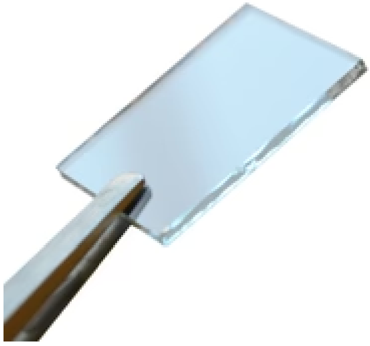
Return to the top



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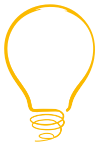

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Return to the top

Return to the top