2.5.1 Curved-grating spectrometer: Wadsworth setup

In a Wadsworth design, a curved grating reduces the number of reflections to two, and the models are often rather small, with a short focal length. The entrance cone is the same as in the other setups described earlier. The grating has a dual function: it disperses the light and refocuses it to the exit slit or a limited field. Because the entrance and exit are opposite each other, rather large periphery can be mounted to relatively small spectrometers. The Wadsworth spectrometer works with two concave reflectors, and thus the angles are limited in variation, and the field is small.

2.5.2 Normal incidence

To cope with declining efficiencies, spectrometers with no mirrors have been designed besides the Czerny–Turner principal. In these cases, the curved grating has a triple function. It is curved to add both mirrors' functions to dispersion. The inclusion angle δ of normal-incidence (NI) instruments is 15 deg or less. Up to this value, the rules of specular reflection are valid. Thus, there will be negligible change in the state of polarization, high area efficiency, and good image transfer. However, spectrometers with short focal lengths offer only a small space between the entrance and exit for adding periphery. Optionally, several NI systems offer a flat deviation mirror (M) between the grating and exit; the unit has one entrance and two exits. The image transfer is not overwhelming, but in most cases it is good enough for line detectors of up to a 12.5-mm width and 2.5-mm height. NI spectrometers work from 30 nm to NIR.

2.5.3 Seya–Namioka

As an alternative, the Seya–Namioka setup can be applied. The entrance and exit are under 70 deg, offering plenty of space to attach accessories or connect to vacuum systems. With the increased δ, the dispersion also increases at the expense of the projected grating surface: at direct reflection, it is down to 66% of the grating's surface, and it will decrease with the grating movement. Furthermore, the grating's curvature needs to be designed for the instrument's angles. Due to the large difference between the entrance and exit angles, shadowing of the grating structure can become a problem because the groove modulation will be shallow. Polarization effects need to be considered at the high angles given. Finally, the transfer function will be poor (except the grating will be corrected), providing a good image for a very limited range of working angles that, in turn, might require a special slit shape. Regardless, imaging applications will be very poor. Seya–Namioka spectrometers are also available down to ~30 nm.

2.5.4 Grazing incidence

In the high-energy range of 1–30 nm (1200–400 eV, soft x ray), the concept of grazing incidence is introduced. The grating will be illuminated with parallel

light under angle $\alpha = 82$–88 deg. The entrance aperture does not have to focus but rather limit the size of the collimated beam. The detector will move on a radius to collect the required set of photon energy. If focusing is required, a hollow metallic mirror will be mounted at the radius and projected at the detector.

2.5.5 Rowland circle spectrometer and Paschen–Runge mount

A spectrometer with two spherical mirrors and a plane grating refocuses the separated wavelengths at the sector of a circle known as the Rowland circle. All wavelengths directed at the circle (and within a certain angular coverage) are well refocused. The method is realized by two different detector arrangements: The detector can travel on a rail and be moved to the wavelength of interest, or, more often, a series of detectors is fixed at the circle to receive a pre-defined wavelength; this was the standard in emission spectroscopy for many years, up to the 1980s. If the grating is concave, the second mirror is obsolete, and the performance is similar but less flexible. That version is named the Paschen–Runge mount. Vacuum-compatible or purged systems have been used routinely for the range of 170–900 nm.

2.6 Other Parameters and Design Features

2.6.1 Straight slits versus curved slits

Spectrometers are optical instruments: they like symmetry. Imagine a straight entrance slit with a 25-mm height; it can be easily understood that rays entering at the upper or lower end of the slit have a longer distance to the center of the grating compared to the rays entering the center of the slit. A calculation at two focal lengths, combining two distances of the slits from the center of the instrument, can help. The focus displacement results from the trigonometric rule, which includes r_1, the radius of the Fastie circle; r_2, the theoretical radius at the end of the straight slit; and d, the distance examined from the slit center. The displacement occurs from the radius and distance to the slit center, not from the focal length, and thus longer-focal-length instruments come with a wider radius to enable larger gratings. The instruments compared (A and B) are as follows:

A. focal length = 1 m (*f*/10); $r_1 = 110$ mm; $r_2{}^2 = (r_1{}^2 + d^2)^{1/2} = ((12100 + 156.25)\ \text{mm}^2)^{1/2} = 110.708$ mm.
B. focal length = 0.3 m (*f*/5); $r_1 = 80$ mm; $r_2{}^2 = (r_1{}^2 + d^2)^{1/2} = ((6400 + 156.25)\ \text{mm}^2)^{1/2} = 80.971$ mm.

The displacement will cause the focus reproduction to deteriorate. Its shape depends on other parameters and angle; in the worst case, it will just add to the slit width (as shown in Fig. 2.22). The error increases from the center to the periphery of the slit, but it is constant at a certain distance and thus causes more difficulties with narrow slits or fine images. At shorter slits, the impact is greatly reduced. For examples A and B, at ±2.5 mm, A = 2.3-μm displacement, and

B = 3.1 μm. Because that size is below the Rayleigh diffraction limit, it will not cause any problems, which is the main reason for limiting the slit height in spectrometers with straight slits.

There are other solutions to this problem. Apart from installing curved slits, which require an axial-symmetric spectrometer design, the slit height used can be reduced until the resolution is acceptable, at the expense of light flux. For imaging spectrometers, optical correction methods are available. (See also Section 2.6.7.5.1 on coma and Section 4.1.6 on output fidelity and correction methods.)

2.6.2 Aperture and light flux (luminosity)

A general equation is used for luminosity or light flux in optical systems:

$$L = A^2 \times T \times \Omega, \tag{2.14}$$

where L is the luminosity (an arbitrary number), A is the illuminated area of entrance and exit of the system, T is the transmission through the instrument at the wavelength under consideration, and Ω is the aperture of the beam. It consists of the active internal area A divided by the square of the focal length, thus taking into account that the light density decreases with the square function of the focal length.

Ω represents the normalized cone angle through the spectrometer; it reflects the fact that the light density (radiance) at a given area drops by the square of distance:

$$\Omega = A_g/f^2, \tag{2.15}$$

where A_g is the illuminated grating area, and f is the focal length that produces the light flux through a spectrometer, described by the arbitrary number L, which allows for the comparison of different instruments for their applicability to a defined experiment.

These parameters are discussed further in Chapter 6. Ω plays a key role in illumination (Section 6.3) and in related applications.

2.6.2.1 Real aperture or *f*-number?

As with a photographic camera, the relation between the active surface and focal length, the aperture, is a measure for the capability of a spectrometer to collect light and guide it to the output (often called the "light-collecting power"). The shorter the focal length and the larger the optical components involved, the more light can be transferred. Also, analogous to other optical systems, the quality of reproduction drops with increasing Ω, which also leads to decreasing spectroscopic performance due to the increasing internal angles of the system. Also note that the chance of getting unwanted light in the output increases.

The aperture is defined by $n = f/Wi$. It is also called the "f-number" or "f-ratio." The light flux in a system of $f/4$ is not twice the light flux of $f/8$: it is $(f/4^2)/(f/8^2)$. A spectrometer with a focal length of $f = 300$ mm and the

capability to illuminate a grating 100 mm wide has $n = 300$ mm/100 mm, or $n = 3$. Unfortunately, by no means it is assured that the grating provides $n = 3$ in real use. Most gratings are rectangular; one with side lengths of 70 mm × 70 mm has a diagonal of roughly 100 mm, but calculations would include nonexistent segments (see Section 2.7.5). Some manufacturers specify the spectrometer as if the areas existed anyway. In other words, if the grating is 100 mm × 100 mm, the diagonal is 140 mm, and some existing segments will remain unilluminated. However, is that really a problem? For both systems, the *f*-number in the datasheet might be the same! It is already known that area losses rise as the grating turns.

Consider a Czerny–Turner with $f = 300$ mm and inclusion angle $\delta = 30$ deg. The grating is 70 mm in width and height, making a diagonal of 100 mm. The mirrors provide some reserve and have a 110-mm diameter. It is obvious that the projected height remains stable as the grating turns, but the width does not. Based on δ, the mirrors are tilted versus the axis by 7.5 deg, producing a loss of cos 7.5 deg, or <1%. The grating "sees" both mirrors at an angle of 15 deg, which creates another loss of 3.5% in both directions, even at zero order. Therefore, it is a good idea to use a wider grating. If it rotates towards the entrance, it reaches full projection at $\alpha = 15$ deg. Above that angle, the illuminated area decreases again. At the illumination angle $\alpha = 45$ deg, it will suffer from 30% loss, at which point only two-thirds of the optimum aperture ($n = 4.5$) are used. If the dispersed light uses the output mirror fully, then the real aperture has been found. If not, the real aperture will be even weaker. Users are advised to not blindly believe the aperture numbers provided by datasheets; rather, they should collect the component sizes and angles, and perform some calculations for planned experiments. The use of Ω will be very helpful—if the Ω of the illumination and the spectrometer are identical, the losses are minimal, and the spectrometric performance is the best.

2.6.2.2 Examples of the influence of the internal angles on the light flux

Consider the following comparison of similar spectrometers with different distances between the collimating and focusing mirror, as well as between the entrance and exit:

- **Center distance = 250 mm**, mirrors and grating are 100 mm × 100 mm, and $f = 500$ mm. The distance between the grating's center to a virtual point between the mirrors is assumed to be 400 mm; with a symmetric ε and a test wavelength of 500 nm, the grating rotates towards the entrance. The theoretical aperture is $n = 5$. For the 25-cm-wide unit, $\alpha = 17$ deg, and $\iota_h = 13$ deg. The projected width of the collimator drops from 100 mm to 97.43 mm. At a 25-cm distance between the beams, $\beta = 44$ deg. Consequently, the projected width at the focusing mirror is 70.1 mm, leading to a working aperture of $n = 7.14$.
- **Center distance = 300 mm**, all other parameters match the previous example, including the theoretical aperture $n = 5$. However, ι_h is now

19 deg, shrinking the effective width of the collimator to 94.55 mm. Also, $\beta = 57.8$ deg, and the projected width at the focusing mirror drops to 53.3 mm. Because the grating itself also has a smaller projection, the total used width becomes 50.4% of the basic size, i.e., a working aperture of $n = 9.9$. In both cases, the used height remains at 100 mm.

In short, there are good reasons to keep a spectrometer as slim as reasonable and to add some experimental reserve to the width of the grating.

2.6.2.3 Calculating the *f*-number versus Ω for light flux/luminosity

Even after exact calculation of the *f*-number n, only half the work is done because the efficiencies of the components at the considered wavelength are not yet provided. Additionally, there is another parameter: the illuminated areas of the entrance and exit.

Unfortunately, the *f*-number is not clearly defined. Knowing the number does not directly lead to the throughput of a spectrometer. On the other hand, the light flux calculation based on Ω does lead to a basis for comparison. The grating area A (the black rectangle in Fig. 2.9), projected from the entrance slit by four solid lines, is calculated. The result is divided by f^2. Between the collimator and grating, the rays travel in parallel fashion, and both areas are the same. The resulting Ω reflects the fact that the light density (irradiance) decreases with the square of the distance. Another advantage of this procedure is that it is fully compatible with the definition of steradian used for illumination. In comparison, *f*-number calculations only regard two linear dimensions: the focal length and one dimension of the illuminated object (mirror, grating).

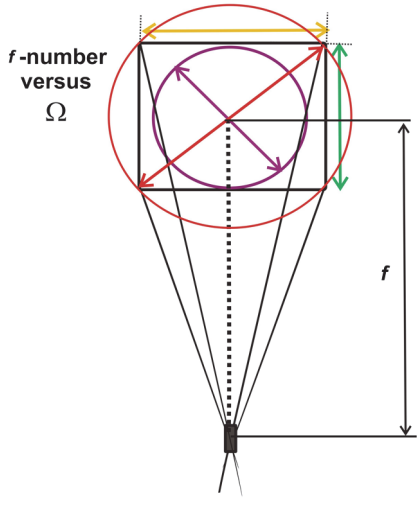

Figure 2.9 Illustration of the *f*-number in comparison with Ω.

The best fit is reached by applying the grating width (marked by the solid dart in Fig. 2.9), which allows for observation of the change of size as the grating turns, which unfortunately is not often applied in datasheets. To compensate for the losses, the actual size of a grating (black frame) should be wider than the height (dotted dart). Sometimes the published *f*-number is based on the inner diameter (light-grey circle), leading to the same result as if the shorter side were used. This scenario presents an *f*-number worse than reality. To present better numbers, some spectrometer vendors define the *f*-number based on the grating diagonal (outer circle, marked dark grey), but this number promises areas of approximately one-third of the theoretical area, which are, in reality, not present. The majority of datasheets do not document which method is used to calculate the *f*-number. To find the correct number, several calculations are required, and thus it is better to use Ω from the beginning.

Therefore, an alternative method is suggested: the calculation of luminosity, or light flux, based on the general equation:

$$L = A^2 \times T \times \Omega,$$

Based on Eq. (2.14), an equation was developed for spectrometers that contains the relevant parameters to estimate the light flux with monochromators and spectrographs. One version allows for prediction with a suitable spectrometer without accounting for the illumination angle. The other version is based on a known cone angle Ω for the light at the entrance. If the irradiance at the entrance slit is known and put into calculations, the quantitative component of the previous version is added. The normalized light-transfer ratio Ω is

$$\Omega = A^2/f^2,$$

where Ω is the normalized light transfer ratio, A^2 is the illuminated or emitting area, and f^2 is the square of the focal length or distance.

The luminosity at the spectrometer output (Fig. 2.10) is found by the following equation:

$$L_s = T \times A_s \times \Omega \times (h_D \times B), \tag{2.16}$$

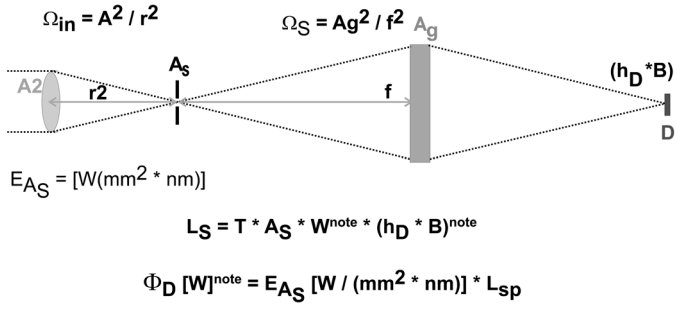

Figure 2.10 The luminosity at the spectrometer output.

where

- T is the transmission of the spectrometer at the wavelength of interest (typically 0.1–0.7). A double spectrometer, comprising identical components, is $T/2$ compared to the single-stage version.
- A_s is the illuminated area of the entrance slit. It is assumed that the irradiance fills the slit completely and uniformly. The dimension is E_{As} = mW/(mm^2 × nm). According to Eq. (2.15), A^2 is the area, assuming that the entrance and exit are of the same size, which is true for monochromators but often not for spectrographs.
- Ω has two meanings. Given as an absolute value, Ω defines the capability of the instrument to collect and transport light, with the radiation traveling in a half-sphere distribution from the slit into the system. However, realistically, the light enters under a defined cone angle, shown in Fig. 2.10 as $A^2/r^2 = \Omega_{in}$. The resulting Ω is the ratio of Ω_S/Ω_{in}, with the result limited to 1 at maximum. In other words, so long as Ω_S is larger than Ω_{in}, all light entering will be transported at the expense of resolution. As soon as Ω_{in} becomes larger than Ω_S, the spectrometer is overilluminated, light will be lost, and even worse, it will create stray light. Hence, it is very wise to adapt Ω_{in} closely to Ω_S, trying to reach a total $\Omega = 1$.
- h_D is the illuminated height in the exit, which can be a slit or a read-out element (pixel or superpixel). It is clear that the maximum height of the exit cannot exceed the height of the entrance. The parameter also includes the radiation that is dispersed at this point. Consequently, the x axis can be defined in millimeters or nanometers, as well.
- B is the spectral bandwidth (nm) in the output slit or at one bandwidth element. The parameter includes the radiation that is dispersed after the grating. The bandwidth results from the dispersion (RD, see Section 2.8.1). If at the time of estimation the bandwidth is not yet known, the geometrical width can be taken. Consequently, the x axis can be defined in millimeters or nanometers, as well.

Note that all calculations negate any kind of aberrations and disturbance—only an ideal system is considered.

The following dimensions are used to calculate a spectrometer regardless of illumination:

$$L_s = T \times A_s[\mathrm{mm}^2] \times \Omega\,[\mathrm{mm}^2/\mathrm{mm}^2] \times (h_D[\mathrm{mm}] \times B[\mathrm{nm}]) = [\mathrm{mm}^2 \times \mathrm{mm} \times \mathrm{nm}],$$

resulting in an arbitrary output parameter that includes height and bandwidth. If, besides the spectrometer, the illumination cone is also known, the two cones (Ω/Ω) are put in relation. If, in addition the irradiance at the entrance is taken into account, we find:

$$L_s = P[\mathrm{W}/(\mathrm{mm}^2 \times \mathrm{nm})] \times T \times A_s[\mathrm{mm}^2] \times \Omega\,[\mathrm{mm}^2/\mathrm{mm}^2]/\Omega\,[\mathrm{mm}^2/\mathrm{mm}^2] \times (h_D[\mathrm{mm}] \times B[\mathrm{nm}]) = [\mathrm{W}].$$