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The use of gratings in the vacuum ultraviolet

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The properties of shperical concave gratings are discussed, with emphasis on applications in vacuum ultraviolet spectroscopy. An expression is derived for the focal curve, which, in general for large radius gratings, deviates appreciably from the Rowland circle. Efficiency and resolution are discussed, and a comparison with laser spectroscopy is made.

1. Introduction

The vacuum ultraviolet (VUV) is the wavelength region below 200 nm. Light of this wavelength is absorbed by air, thus experiments in this region have to be performed in vacuum. There are also a few transparent media, down to 105 nm, comprising only a few solids, e.g., LiF and MgF and the rare gases, which are transparent above limits between 50 and 100 nm. Often the VUV region is subdivided into the Schumann- or VUV-region above 100 nm and the extreme ultraviolet (XUV) below 100 nm. In the lowest part, below 20 nm, the VUV overlaps with the soft X-ray region and here both optical and X-ray methods can be applied.

The lack of transparent materials causes optical systems for these wavelengths to be made with reflective components. Also reflectivity becomes poorer when going to lower wavelengths and this means that usually one wants to use as few optical elements as possible. So, generally a spectrograph or monochromator consists of a concave spherical grating in a mounting based on the Rowland circle. In this way, the number of reflections is minimized. In the wavelength region below 50 nm, the reflectivity of all materials is down to only a few percent and one has to use a grazing incidence mounting to take advantage of the fact that the reflectivity approaches unity at very large angles of incidence.

2. Focusing properties of the spherical concave grating

The theory of the spherical concave grating is treated by different authors [1]–[3]. BEUTLER [3] used in his well-known paper the principle of Fermat, which was first applied to this problem by ZERNIKE [2]. This method is in principle as follows. The optical path (see Fig. 1) is defined by

$$F = AP+BP+Nk\lambda. \tag{1}$$

The last term arises because an integral number of wavelengths increases when we go from one groove to the next. Now, AP and BP are expressed in polar coordinates and expanded in a power series. This leads to an expression for the optical path

$$F = F_1+F_2+F_3+F_4+F_5+F_6+\dots \tag{2}$$

where each term has a well-defined physical meaning.

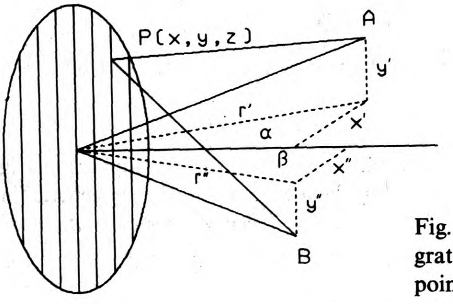

Fig. 1. Principle of Fermat applied to the spherical concave grating. $A(x', y', z')$ is a source point, $B(x'', y'', z'')$ is an image point, and $P(x, y, z)$ is a point on the surface of the grating

If we now apply the Fermat principle to the first two terms we find the grating equation, and respectively the focusing condition. We have to take the derivatives of the pathlength with respect to a change in the position of $P(x, y, z)$. The complete expression for the first terms is

$$F_1 = r'-y\sin\alpha+r''-y\sin\beta+Nk\lambda. \tag{3}$$

If we take the derivative of this expression with respect to y, and equate this to 0, we find (remember that $N = y/d$)

$$\sin\alpha+\sin\beta = k\lambda/d, \tag{4}$$

the well-known grating equation.

In the same way we find the focusing condition by requesting that the derivative of F_2 equals 0 for all values of y

$$\mathrm{F}_2 = \frac{y^2}{2}\left[\frac{\cos^2\alpha}{r'}-\frac{\cos\alpha}{R}+\frac{\cos^2\beta}{r''}-\frac{\cos\beta}{R}\right]. \tag{5}$$

This leads to

$$\frac{\cos^2\alpha}{r'}-\frac{\cos\alpha}{R}+\frac{\cos^2\beta}{r''}-\frac{\cos\beta}{R} = 0. \tag{6}$$

The so-called self-focusing curve (i.e., the curve where both r' and r'' are defined in the same way and fulfil (5)) is the Rowland circle, defined by

$$r' = R\cos\alpha. \tag{7}$$

If, however, the groove distance is not constant across the grating (which was assumed but (almost) never is the case in practice), but varies slowly across the grating, then we can assume that to first order the groove distance is given by

$$d = d_0(1+gy) \tag{8}$$

where d_0 is the groove distance in the centre of the grating ($y = 0$) and g is a constant. We now find

$$\frac{dy}{dN} = d = d_0(1+gy) \tag{9}$$

and integration gives

$$N = (y/d_0)(1+gy/2). \tag{10}$$

If we insert this expression in (3), we find an additional term in the derivative of F_1 which depends on y. We add this term to the derivative of F_2 which also depends on y. In this way, the total change in the light path function remains 0. Also the grating equation remains unchanged. In this way (5) is replaced by

$$\frac{\cos^2\alpha}{r'} - \frac{\cos\alpha}{R} + \frac{\cos^2\beta}{r''} - \frac{\cos\beta}{R} - g\frac{k\lambda}{d_0} = 0. \tag{11}$$

We substitute the grating equation in the rightmost member of the left-hand term and define a new constant

$$e = g/R. \tag{12}$$

The self-focusing curve now becomes

$$r' = \frac{R\cos^2\alpha}{\cos\alpha + e\sin\alpha}. \tag{13}$$

Already in 1893 CORNU [1] derived this result using geometrical arguments. At the Zeemanlaboratorium we have tested seven large gratings with radius of curvature about 6.65 m [4], and found that the value of g varied from 0.46×10^{-7} to $0.3\times10^{-5}\ \mathrm{mm}^{-1}$. Under these circumstances the distance between the Rowland circle and the real focal curve was of the order of several centimeters in the directions where these gratings were actually used (see Fig. 2).

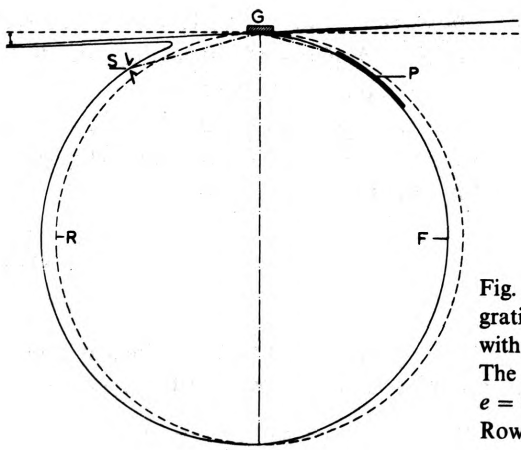

Fig. 2. Self-focusing curve for a spherical concave grating with a non-constant groove spacing, compared with the Rowland circle, in a grazing incidence mounting. The curve given here is for a hypothetical grating with $e = 0.1$ (G – grating, S – slit, P – plateholder, R – Rowland circle, F – focal curve)

3. Aberrations of the spherical concave grating

The remaining terms have then the following meaning:

astigmatism

$$F_3 = \frac{x^2}{2}\left[\frac{1}{r'} - \frac{\cos\alpha}{R} + \frac{1}{r''} - \frac{\cos\beta}{R}\right] - \frac{xz'}{r} + \frac{z'^2}{2r'} - \frac{xz''}{r''} + \frac{z''^2}{2r''},$$

coma and line curvature

$$F_4 = \frac{x^2 y \sin\alpha}{2\ r'}\left[\frac{1}{r'} - \frac{\cos\alpha}{R}\right] + \frac{y\sin\alpha}{2r'^2}(2xz' + z'^2) + \frac{x^2 y \sin\beta}{2\ r''}\left[\frac{1}{r''} - \frac{\cos\beta}{R}\right] + \frac{y\sin\beta}{2r''^2}(-2xz'' + z''^2),$$

spherical aberration

$$F_5 = \frac{(x^2+y^2)^2}{8R^2}\left[\frac{1}{r'} - \frac{\cos\alpha}{R} + \frac{1}{r''} - \frac{\cos\beta}{R}\right].$$

F_6 vanishes under focusing conditions on the Rowland circle. We shall now discuss these terms in brief.

An important aspect of the use of spherical concave gratings is some appreciable amount of astigmatism inherent in these optical systems. In the plane of the focal curve a point of the slit is imaged as a point but, in the perpendicular direction, a point is imaged as a point only when it is at a distance from the slit given by

$$s = R[(\cos\alpha - \sin\alpha\tan\beta)^{-1} - \cos\alpha]. \tag{14}$$

A point on the slit is perpendicular to the focal plane, imaged as a line of length

$$z'' = l(\sin^2\beta + \sin^2\alpha\cos\beta/\cos\alpha) \tag{15}$$

where l is the length of the grooves of the grating. This astigmatism can cause loss of light, when not compensated for, and is very important for grazing incidence mountings, where the angles α and β are large. Coma can be neglected when the focusing curve is not far from the Rowland circle and also line curvature does not play a very important role as long as we do not come too close to the grating. Spherical aberration can present more of a problem, especially at grazing incidence. The only way to control this aberration is to limit the term F_5 to a quarter of a wavelength. This leads to a maximum grating diameter given by

$$W_{\text{opt}} = 2.38\left[\frac{\lambda R^3 \cos\alpha\cos\beta}{(1-\cos\alpha\cos\beta)(\cos\alpha+\cos\beta)}\right]^{1/4}. \tag{16}$$

At grazing incidence were both the wavelength and the geometrical factor are small, the useful width of a grating is restricted to a few centimetres even at large radius of curvature.

4. Efficiency of gratings

One should always keep in mind that the efficiency of a grating changes with wavelength. Most gratings are blazed, which means that the groove shape has been optimized for a certain wavelength. Particular parameters of a mounting can shift this blaze wavelength to some extent. For the general change in efficiency see Fig. 3.

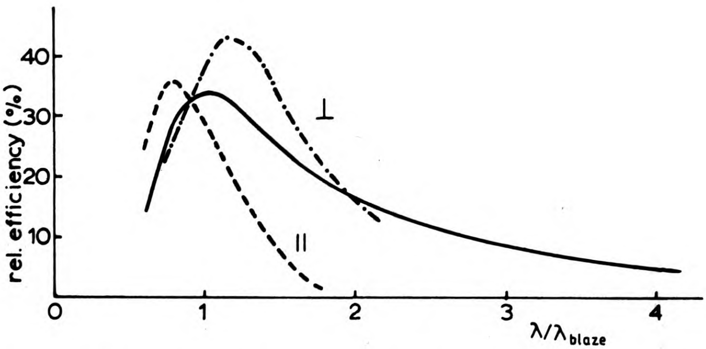

Fig. 3. Efficiency curves for a grating, the deshed lines represent polarized light

The solid curve gives the average value for light polarized parallel and perpendicular to the grooves. The efficiencies for these two polarization states usually differ from each other. This means that a grating can act as a polarizer. In the VUV, the usual monotonous decrease in reflectivity increases this curve on the long wavelength side and decreases it on the short wavelength side, but the overall picture remains.

Intensity anomalies can cause difficulties, especially if they change the grating efficiency over short wavelength intervals. The most common are the so-called Wood's anomalies, which occur for wavelengths given by

$$k_R \lambda_R = d(\sin\alpha \pm 1). \tag{17}$$

They often give rise to abrupt changes of the intensity and can be different for light polarized perpendicular or parallel to the grooves.

5. Resolving power

The resolving power of a spectrograph is determined by the following three factors:

1. The resolving power of the grating, given by the formula

$$R_g = kN \tag{18}$$

with k – the spectral order and N – the number of grooves of the grating.

2. The resolution of the photographic plate Δs (typical of the order of 10 μm)

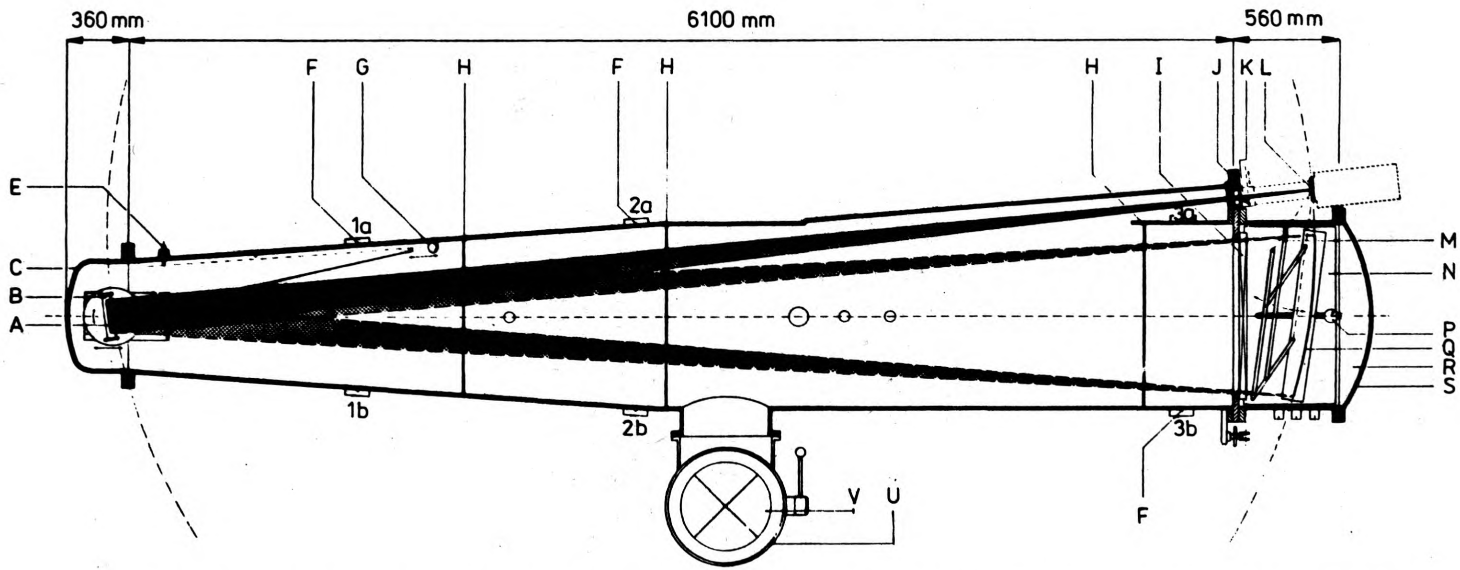

Fig. 4. Normal incidence vacuum spectrograph at the Zeemanlaboratorium. A – grating, B – grating holder containing two gratings, C – cover, E – adjusted photomultiplier, F – thermocouples, G – photomultiplier, H – light baffles, I – vacuum valve between photographic chamber and main tank, J – valve between slit and main tank K – movable mirror, L – slit, M – plateholder mounting, N – support for plateholder, P – measuring device for position plateholder, Q – photographic plates, R – photographic chamber, S – lid of photographic chamber, U – diffusion pump, and V – vacuum valve

which results in a resolution of

$$\Delta\lambda = \frac{\lambda\cos\beta}{R(\sin\alpha+\sin\beta)}\Delta s \tag{19}$$

which is in fact the resolution of the plate multiplied by the so-called platefactor, the inverse of the linear dispersion.

3. The width of the slit.

The resolution resulting from all these factors produces a lineshape formed by the convolution of the shapes resulting from each of these factors.

For high resolution one needs spectrographs with a high dispersion, for otherwise the second factor will limit the performance of the instrument.

6. Large vacuum spectrographs

There are only a limited number of laboratories which cover the whole VUV wavelength range with spectrographs with high resolution. The National Bureau of Standards in Gaithersborough near Washington, D. C., the Spectroscopic Laboratory of the Academy of Sciences of the USSR in Troitzk near Moscow, and the Zeemanlaboratorium in Amsterdam should be mentioned in this respect. The instruments in the Zeemanlaboratorium will be discussed as typical examples of high performance spectrographs in the VUV.

A schematic picture of the normal incidence spectrograph [5] is shown in Fig. 4. Due to recent improvements, this instrument has been equipped with two gratings mounted in a system which allows us to exchange them and to change wavelength range in a few minutes. This system also allows us to maintain a perfect adjustment without any refocusing even for more than a year. The characteristics of the gratings are given in the Table. This spectrograph can be used in the wavelength range of 2300–400 Å. Its resolving power is given in the Table.

Theoretical resolving power of the 6.6 m normal incidence spectrograph at the Zeemanlaboratorium in first order, assuming a resolution of the photographic plane of 10 μm

Grating	Wavelength	Resolving power
	200 nm	167000
1200 grooves/mm	160 nm	133000
	120 nm	100000
	120 nm	200000
2400 grooves/mm	800 nm	133000
	400 nm	67000

The grazing incidence spectrographs [6] is shown in Fig. 5. This instrument is equipped with a gold coated grating with 1200 grooves per mm. The grating is only 80 mm wide and 20 mm high. Astigmatism makes longer grooves useless and

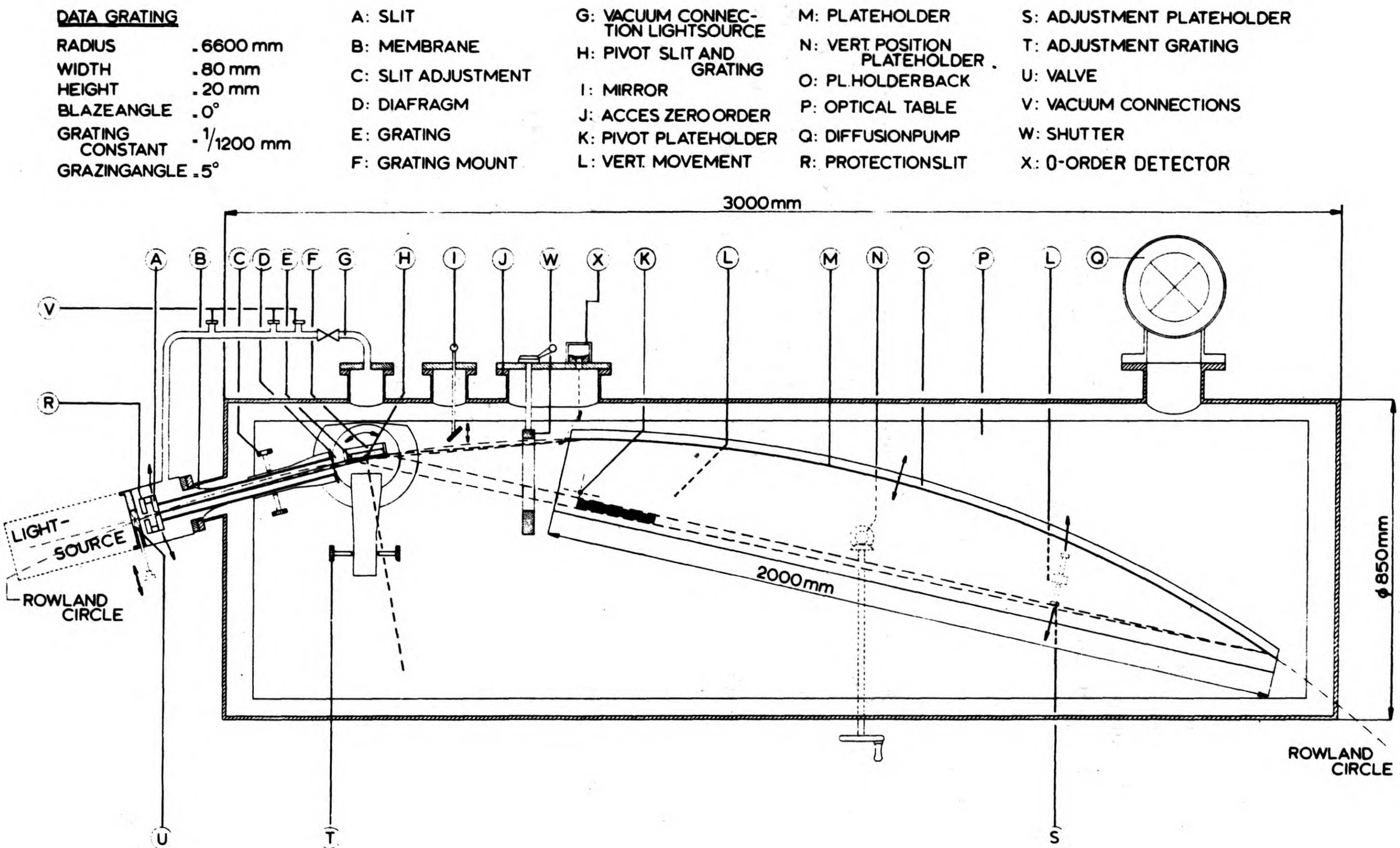

Fig. 5. Grazing incidence spectrograph at the Zeemanlaboratorium

spherical aberration prevents the use of a wider grating. At shorter wavelengths we have even to screen part of the grating to get an optimum resolution. The resolving power is given in Fig. 6.

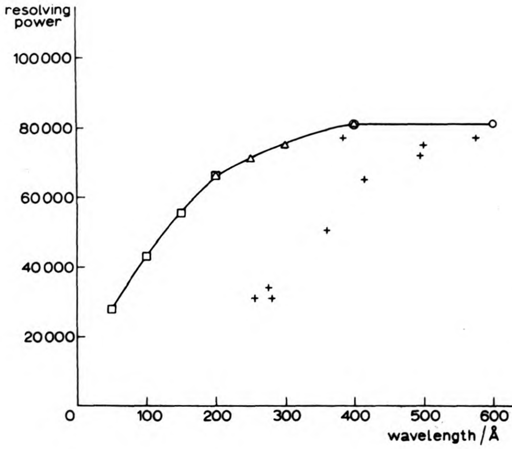

Fig. 6. Resolving power of the grazing incidence spectrograph. Theoretical resolving power limited by: o — the maximum grating width, △ — the optimum grating width, □ — the resolution of the photographic plate (10 μm), + — the practical resolving power obtained

7. Concluding remarks

In the visible and ultraviolet wavelength regions, dispersive spectroscopy — where one uses a grating of prism as wavelength selective element — is nowadays largely replaced by laser spectroscopy, except for analytical purposes. There are several reasons which make a similar development unlikely in the VUV. The lack of transparent media makes the construction of an easy-to-handle laser very difficult and also the production of coherent radiation by frequency doubling or by related methods is not so easy. In addition, the tuning range is very small without rebuilding the experimental setup. Furthermore, laser spectroscopy is essentially an absorption technique and contrary to the situation in the visible and ultraviolet, the transitions in the VUV are mainly ionic transitions. Only the rare gases and hydrogen form an exception. This means that one has to prepare multiply-ionized atoms as an absorption medium and that is a complicated task.

In the VUV, dispersive and laser spectroscopy will probably remain complementary techniques, where grating spectrographs will provide a general overview of a large wavelength region and laser spectroscopy will be used only for the study of specific details at very high resolution.

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Применение сеток в ультрафиолете в вакууме

Продискутированы свойства сферической вогнутой сетки с осбенным хажимом на применение в вакуумной спектроскопии в ультрафиолете. Введены уравнения для фокусной кривизны, которые для сеток с большим радиусом отклоняются в значительной степени от круга Ровланда. Продискутированы производительность и распределительность, совершено также сравнение, опираясь на лазерную спектроскопию.