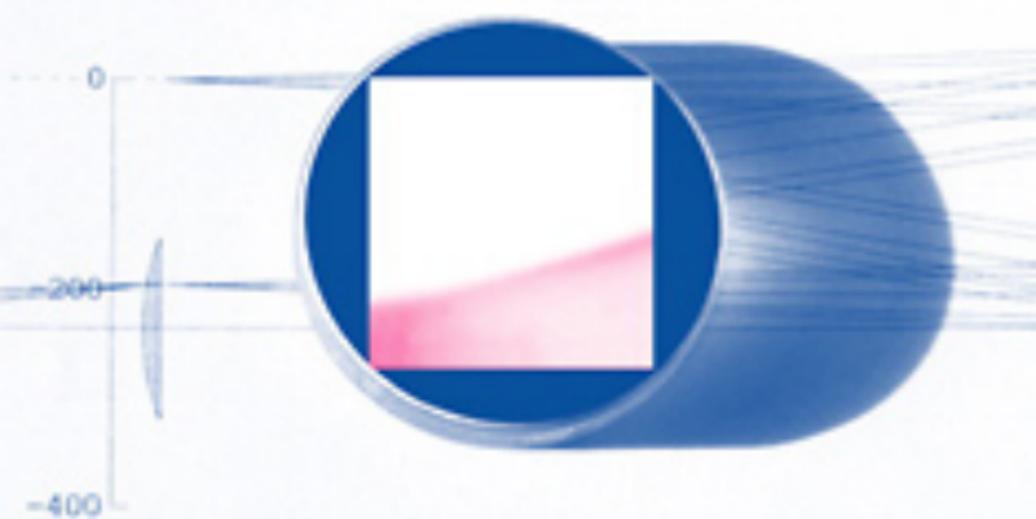


# Spectrograph Design Fundamentals



**John James**

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## SPECTROGRAPH DESIGN FUNDAMENTALS

In recent years enormous changes have occurred in the field of optical spectrometry. The classical spectrometer has become obsolete and the spectrograph, in combination with the CCD detector, now offers a vastly superior approach. Although the basic optical principles remain unchanged the design considerations are very different, and in many cases more demanding. However, developments in computer ray-tracing and computer-aided design have coped with these extra impositions and have allowed the construction of a new generation of spectrographs.

The book covers the general principles of spectrographic design, and the practical and engineering aspects of a broad range of spectrographs and spectrometers. This allows the reader to make an informed choice of instrument. It will be of particular use when none of the immense array of manufactured spectrographic and spectrometric instruments is suitable for a specialised task. The book deals with materials and methods of construction and includes suggestions for the choice of optical table, the design of slit mechanisms, and adjustable mirror, grating and lens mounts, with suggestions for the alignment and calibration of the finished instrument.

*Spectrograph Design Fundamentals* describes the design and construction of optical spectrographs. It will be a valuable resource for academic researchers, graduate students and professionals in the fields of optics, spectroscopy and optical engineering.

JOHN JAMES is an Honorary Senior Research Fellow at the University of Glasgow and a Fellow of the Royal Astronomical Society. He is the author of *Student's Guide to Fourier Transforms*, also published by Cambridge University Press, now in its second edition.



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## Preface

Thirty-eight years ago, together with my colleague the late Robert Sternberg, I wrote a book entitled *The Design of Optical Spectrometers*. It described the state of the art as it was at that time after the great advances which had come in the previous ten years, and it was intended for people who wished to build a spectrometer tailored to a specific purpose, where perhaps one of the commercial designs was inadequate, unsuitable, unnecessarily cumbersome, or expensive.

When at last the time came to consider a new edition it became clear that the technology had changed so much that the classical optical spectrometer, in the sense of *monochromator*, was more or less obsolete and that later developments such as the desktop computer and the charge-coupled device had restored the spectrograph to its former eminence. The restoration in no way annulled the optical improvements of the previous 30 years but new constraints posed new problems in design. These problems are now solved and the solutions are presented here.

The fundamentals of optical design have not changed, but the constraints are now all different, and such properties as flat fields are needed where before they could be largely ignored; and focal ratios matter again when previously we could design everything so that such trivia as spherical aberration and coma could be neglected.

There is, as always, a gap to be bridged between the elegant theory presented in the undergraduate textbooks and the practical spectroscopic instrument standing on the laboratory bench or bolted to the Cassegrain focus of an astronomical telescope. The gap is partly in the limitations imposed by the curse of non-linearity in geometrical optics and the contumacious aberrations it produces, and partly in the sometimes obstinate physical properties of the materials of construction. As always in scientific instrument making, the art is in knowing what must be precise and exact and what can be left go hang at a crude level. There are tricks in this trade just as in any other. The traditional engineer's description of a physicist is 'someone who designs a box that must be screwed together from the inside'. (There is a parallel physicist's definition of an engineer: someone who, when asked 'what

is three times four?’ will get out a slide rule and answer ‘about twelve’.) There is an element of truth in this and some of the hints in these pages may help to refute the calumny.

This work is thus intended for the new generation of researchers who desire high efficiency in an instrument tailored to their own particular purpose, and who have access to a mechanical workshop of moderate size where an instrument of their design can be constructed. There has been no attempt to venture into the new fields of optical resonant scattering spectroscopy, tunable laser spectroscopy or other specialised techniques and so the book is directed to chemists, astronomers and aeronomers as much as to physicists.

Manufactured spectrographs are in no way deficient, but are necessarily compromises, both in performance and cost, and are often intended for teaching or dedicated to a routine task such as sample analysis. A specially designed instrument has no difficulty in excelling them for a particular investigation, particularly in academic research fields where new areas are being explored and where no established technology yet exists.

It is to the basic optical design and construction of such individual instruments that this book is dedicated. I also take the opportunity of acknowledging my late good friends and colleagues, Dr H. J. J. Braddick, Rob Sternberg and Larry Mertz, from whom I learned so much.

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# 1

## A brief history of spectroscopy

The earliest reference to optical spectroscopy that we have in modern times appears to be the *phenomenon of colours* in Isaac Newton's *Opticks*, in which he describes his famous experiments with prisms and the shaft of sunlight coming through the hole in his window shutter. There was much philosophical conjecture at the time but scientific silence from then on until William Hyde Wollaston (1766–1828) in 1802, also in Cambridge, used a lens to focus images of a narrow, sunlight-illuminated slit through a prism on to a screen. Wollaston appears to have observed the dark lines across the spectrum transverse to the dispersion direction but ascribed them to the divisions between the colours. He may be forgiven for this, because with a single lens the spectral resolution would have been derisory. At about the same time William Herschel (1738–1822) discovered the infra-red radiation by the rise in temperature of the bulb of a thermometer when he held it beyond the red part of the spectrum in his spectroscope. Joseph von Fraunhofer (1787–1826) saw more dark lines but did not guess or deduce their origin. The currently accepted explanation – the absorption of continuous white light by vapours in the atmosphere of the Sun – was given by Gustav Kirchhoff and Robert Bunsen in the University of Heidelberg who, we may be reasonably certain, passed a collimated beam through their prism before focusing it, and thereby secured a reasonable resolution. It is probably to these two but perhaps to Fraunhofer as well that we owe the classical form of the optical spectroscope: the sequence of collimator, prism and telescope. Little has changed fundamentally since then.

Developments in geometrical optics kept pace with developments in photography. From Lord Rayleigh we have the complete theory of the prism spectroscope and of the diffraction grating. Comparatively crude but useful diffraction gratings could be ruled on the bed of any screw-cutting lathe and many individual workers made gratings for their own use, but without passing on the art. Practical details of grating construction were given by R. W. Wood of Johns Hopkins University. At this stage though, they were little more than scientific curiosities emphasising the

wave nature of light. This was at a time when the corpuscular theory was by no means dead.

However, diffraction gratings were first realised at a serious and practical level by H. A. Rowland, also of Johns Hopkins University, who first devised ruling engines capable of the necessary precision.

The prism spectroscope continued in its role as the chief instrument of astronomical botany – the taxonomy or classification of stars, that is – but the resolution available then was insufficient to do more than measure wavelengths, identify and discover elements and to allow wise comments on the mysterious ‘fluted’ spectra sometimes found in flames as well as in cool stars, so described by their resemblance, at low dispersion, to the flutings on the columns of classical temples. It was a major achievement for a spectroscope to be able to resolve the six angstroms separating the ‘D’ lines of sodium, and Rayleigh computed that a prism base length of ‘at least 1 centimetre’ would be needed for this, that is to say a resolving power of  $\sim 1000$ .

Sir Arthur Schuster achieved a resolving power of more than 10 000 at Manchester University with a twelve-prism<sup>1</sup> spectroscope made for him by Cooke of York, with 30 glass–air interfaces (excessive even in a modern coated zoom lens!) and prism bases of 25.4 mm. With incidences near the Brewster angle there should have been near perfect transmission for one state of polarisation, but in practice a transmission coefficient of about 0.05 made it virtually useless except as a sort of tour de force of the spectroscope-maker’s art. The way forward in those days was the manufacture of ever-larger prisms from ever-denser glasses.

The finely ruled diffraction grating by contrast improved the spectral resolution immeasurably and led to the evolution of the spectrograph at the hands of H. Ebert, who in 1889 removed chromatic aberration and a great deal more besides by replacing the lenses of the collimator and the camera with a single concave mirror. The symmetry was intended to eliminate coma as well as chromatic aberration but the apparent symmetry is removed by the tilt of the grating and, although reduced, the coma is still there.

Ebert’s invention was inexplicably lost until rediscovered by W. G. Fastie 50 years later, by which time the single mirror had been replaced by two separate mirrors in the now standard Čzerny–Turner configuration.

It was the invention of efficient vacuum pumps which led to the investigation of gas-discharge phenomena by Crookes and others and the consequent exploration of gaseous emission line spectra. This led in turn to the empirical discoveries by Balmer, Paschen and Rydberg which gave rise to the need for an explanation and the consequent invention of the Bohr model of the atom and the subsequent evolution of quantum mechanics.

<sup>1</sup> In practice six prisms each passed twice.

In the twentieth century the spectroscope developed in accordance with the best detector technology available at the time. Little happened before 1950 in the optical part of the spectrum although infra-red detectors made considerable progress, and at wavelengths below  $0.8\ \mu\text{m}$  the photographic emulsion was the universal detector, the spectroscopic art advancing along with improvements in its sensitivity and panchromaticity. By *c.* 1950 the whole electromagnetic spectrum from soft X-rays to about  $1.2\ \mu\text{m}$  was available to silver halide emulsions and the short-wave limit to practical spectrography was set by the reflection coefficients of the optical components, which were – and are – dismal below about  $1200\ \text{\AA}$ . This limitation was offset by the gradual development of improved sources of XUV light such as the synchrotron for absorption spectrography and later spectrometry.

Semiconductor detectors improved the accessibility of the infra-red, and the photomultiplier, which became generally available *c.* 1950, revolutionised optical spectroscopy. This device yielded a detective quantum efficiency (DQE) in the region of 0.2–0.35 as opposed to the DQE of a silver halide crystal of about 0.0005 and, just as importantly, gave a linear response.<sup>2</sup> One of the bugbears of the silver halide emulsion, especially at the low surface brightness of many astronomical sources, was *reciprocity failure*, the inability to respond adequately to long exposures at a low light level. Consequently a monochromator with a photomultiplier detector, free from the constraints of low focal ratio, could easily out-perform a spectrograph and moreover could be made to concentrate its efforts on the parts of the spectrum important to the investigation being made.

Geometrical optical design was then brought to bear, resulting not only in high efficiency but in much greater resolving power, sometimes reaching 80–85% of the theoretical level imposed by the constraints of physical optics.

In parallel with the development of the grating spectrograph, interference spectrometry extended the high-resolution end of the art. Rayleigh again observed that the signal from a Michelson interferometer was the Fourier transform of the spectrum of the incoming light but little note was taken of it at the time except as a scientific curiosity, and it was Charles Fabry and Alfred Pérot in the University of Marseille who in 1899 devised the interferometer which revealed fine and hyperfine structure in spectral lines. Other simultaneous devices, such as the echelon grating,<sup>3</sup> the Lummer plate<sup>4</sup> and the échelle<sup>5</sup> gave equally high resolution but were far less convenient to use and were not widely copied. In the visible and UV region it is the

<sup>2</sup> Based upon the experimental finding that  $\sim 1000$  photoelectrons must be liberated within a microcrystal of silver bromide, irrespective of its size, to make it developable.

<sup>3</sup> A. A. Michelson, *Astrophys. J.*, **8** (1898), 37.

<sup>4</sup> O. Lummer, *Verh. Deutsch. Phys. Ges.*, **3** (1901), 85.

<sup>5</sup> G. R. Harrison, *J. Opt. Soc. Amer.*, **39** (1949), 522.

Fabry–Perot interferometer in its various guises which still rules the high-efficiency end of the spectrographic art.

Meanwhile high resolution was being achieved by more-or-less heroic means, with plane-grating instruments of two or three metres focal length and focal ratios of F/20 or F/30. This ensured at least that the optical resolution would be diffraction limited and that photographic exposures would take an inordinately long time. Academic research was simultaneously being carried out using concave gratings of up to ten metres radius, in spectrographs which filled a whole room in a laboratory or the whole of the Coudé focus room of a large astronomical telescope. There appears to have been some confusion at the time between *dispersion* and resolution, as though one depended on the other, and dispersion itself was taken as a measure of quality or performance. With the passage of time has come improved knowledge and a spectrograph much bigger than one metre or perhaps two in focal length is now a rarity. Provided that an adequate design is chosen, all the information that can be extracted from a spectrograph can be revealed with a 1.5-metre instrument.

The period between 1950 and 1970 saw a great surge in activity in the art of optical spectroscopy. This followed Jacquinet's revelation that 'L-R product' or 'efficiency' in a spectrometer, defined as the product of 'throughput' or 'light-grasp'<sup>6</sup> and resolving power, was a constant and that one quality could be traded for the other. There was consequently a huge blossoming of ingenious, weird and wonderful inventions, including the mock-interferometer,<sup>7</sup> the Sisam,<sup>8</sup> the Girard grille,<sup>9</sup> the Möbius-band interferometer,<sup>10</sup> the tilting Michelson interferometer,<sup>11</sup> the lamellar grating interferometer<sup>12</sup> and various 'chirped' and field-compensated Michelson Fourier spectrometers.<sup>13</sup> Much time and effort were expended to bring these ideas to practical use and the two famous 'Bellevue' conferences of 1957 and 1967 brought all these people together for an exchange of ideas.

However, this insubstantial pageant has faded and very few of the devices described there have survived the test of time–convenience–cost-benefit analysis.

The concept of L-R product is important, indeed fundamental. The idea of resolving power, defined as  $R = \lambda/\delta\lambda$  where  $\lambda$  is the wavelength being observed and  $\delta\lambda$  the smallest wavelength separation that can be distinguished as two separate

<sup>6</sup> A felicitous phrase from H. A. Gebbie.

<sup>7</sup> L. Mertz, N. O. Young & J. Armitage, *Optical Instruments and Techniques*, K. J. Habell, Ed. (London: Chapman & Hall, 1962).

<sup>8</sup> Spectromètre Interférentiel à Sélection par l'Amplitude de Modulation. P. Connes, *J. Phys. Rad.*, **19** (1958), 197.

<sup>9</sup> A. Girard, *Opt. Acta*, **7** (1960), 81.

<sup>10</sup> W. H. Steel, *Opt. Acta*, **11** (1964), 211.

<sup>11</sup> R. S. Sternberg & J. F. James, *J. Sci. Instrum.*, **41** (1964), 225.

<sup>12</sup> J. D. Strong & G. A. Vanasse, *J. Phys. Rad.*, **19** (1958), 192.

<sup>13</sup> L. Mertz, *J. Opt. Soc. Am.*, **49** (1959), iv; P. Bouchareine & P. Connes, *J. Phys.*, **24** (1963), 134; Y. P. Elsworth, J. F. James & R. S. Sternberg, *J. Phys. E*, **7** (1974), 813.

spectrum lines, is an old, dimensionless quantity and a useful parameter of quality in a spectroscope. ‘Light grasp’ on the other hand, also known as ‘luminosité’ or ‘étendue’ and generally denoted by the letter  $L$ , is less familiar and is a measure of the rate at which an optical instrument can process the power it receives from the incident electromagnetic field. It can be defined as the product of detector sensitive area and the solid angle subtended by the detector at the exit pupil of the system<sup>14</sup> or alternatively as the product of the area of the exit pupil and the solid angle subtended by the detector sensitive area. Both of these definitions are derived from the *Helmholtz–Lagrange* invariants of the system. The constancy of the product can be envisaged easily by referring to a simple prism spectroscope. If the entry-slit width is doubled, twice as much light passes through but the resolution is halved.

The concept is much more universal than this and it became apparent that high-resolution devices such as the Fabry–Perot interferometer, possessing a much higher  $L$ - $R$  product than a grating spectrometer, could be used at moderate resolution to examine low-luminosity sources. Soon afterwards the ‘multiplex’ or Fellgett<sup>15</sup> (so named after its discoverer) advantage made Fourier-transform spectroscopy with a Michelson interferometer a highly desirable goal despite its formidable technological problems – now happily solved.

For more than 30 years the monochromator in one form or another ruled supreme until it was rudely overthrown by the arrival of the charge-coupled device, the ‘CCD’. When cooled to the temperature of liquid nitrogen the CCD has a detective quantum efficiency of  $\sim 0.5$  or more and it is, in effect, a photographic plate with an ISO rating in the region of 3 000 000 and a resolution of anything up to 100 line-pairs/mm.<sup>16</sup> The other improvements which it brought are legion: the lack of reciprocity failure, the enormous dynamic range in the region of 50 000,<sup>17</sup> the virtually instant read-out on to a computer screen, and so on. To develop its full potential in spectrography it has been necessary to return to geometric optics in spectrograph design, as there is a strict requirement for a flat field, and a distinct advantage in a low focal ratio; and there are modern advances which would have benefited the Victorian spectrograph had the problem been tackled at the time.

<sup>14</sup> Which for  $F$ -numbers  $\geq 1.5$  is related to the focal ratio  $F$  by  $\Omega = \pi/4F^2$ .

<sup>15</sup> P. Fellgett, *J. de Phys.*, **19** (1958), 187, 237.

<sup>16</sup> As compared with the fastest and consequently coarsest silver halide emulsions with ISO ratings in the region of 2000 and  $\sim 50$  line-pairs/mm.

<sup>17</sup> Silver halide has a dynamic range of about 100: it saturates at  $\sim 100$  times the minimum exposure needed to produce blackening.

## 2

### The relevant regions of the electromagnetic spectrum

The extent of the electromagnetic spectrum is too well known to require description here. We shall be chiefly concerned with the so-called ‘optical’ region, of which the boundaries are determined partly by the methods of detection and partly by the methods of dispersing and analysing the radiation. What is common to all parts of the region is the type of optical element and materials of construction of spectroscopic instruments. Beyond the region on the long-wave side, coherent detectors, paraboloidal aerials, waveguides and dipole arrays are used, and on the short-wave (X-ray) side, optical elements other than diffracting crystals and grazing incidence reflectors are generally unknown. Radiation of  $100 \text{ \AA}$  wavelength liberates photoelectrons with more than 100 eV of energy and the appropriate detection methods are those of radiography and nuclear physics.

Broadly we can identify six wavelength divisions appropriate to optical design techniques:

- 50–15  $\mu\text{m}$ . The far infra-red (FIR), where bolometric, superconductor and semiconductor detectors are the chief methods of detection and measurement, and only specialised materials such as selenium, thallium bromide and various polymer resins such as sulphones have the necessary transparency to make useful refracting components. Optical elements may well be polymer plastics of high dielectric constant. Reflecting elements are coated with gold. New FIR-transparent materials with desirable optical properties are appearing all the time. Nevertheless, the principles of design which make use of them are unchanging and it is important to pay attention to their refractive index and partial dispersion or  $\nu$ -value when deciding whether to use them.
- 15–1.2  $\mu\text{m}$ , 0.1–1 eV. The near infra-red, where there are many suitable refracting materials, and where semiconductor, superconductor and bolometric detectors prevail. This region includes the two ‘windows’, the 2–4  $\mu\text{m}$  band and the 8–13  $\mu\text{m}$  band where the atmosphere is transparent. The opacity does not much concern laboratory work, but is important if aeronomy, telecommunications or astronomical research is in view. The edges

of the regions, where absorption is slight but noticeable, are particularly difficult regions to work in.

- 1.2–0.35  $\mu\text{m}$ , 12 000–3500  $\text{\AA}$ , 1–3.5 eV. The near infra-red, visible and near ultra-violet (UVOIR)<sup>1</sup> region where both semiconductors, photoconductors, photochemical reactions and photoemitters can be used, the latter directly as so-called ‘photon-counters’ (in reality photoelectron counters). This, not unnaturally, is the best understood region of the spectrum and where the greatest variety of refracting materials are known. It is also the region between 1 eV and 3 eV of energy, where interesting things happen in chemistry and physics, where atoms and molecules display their properties, where chemical reactions take place. At wavelengths above 8000  $\text{\AA}$  atmospheric transmission is patchy with extensive regions of opacity caused by water-vapour and oxygen molecules. Laboratory work is unaffected but aeronomers, astronomers and surveyors may have problems when they need long path lengths through the atmosphere.
- 0.35–0.20  $\mu\text{m}$ , 3500–2000  $\text{\AA}$ , 3.5–6 eV. The far ultra-violet, where optical components must be selected carefully for adequate transmission<sup>2</sup> and phosphors are required to convert the radiation into longer wavelengths for registration by optical detectors. Again laboratory work is unaffected but the ozone layer of the atmosphere at 45 km effectively absorbs all extra-terrestrial UV radiation below 2900  $\text{\AA}$ . Laboratory sources emitting these wavelengths (a quartz-envelope mercury vapour lamp for example, which emits the 2537  $\text{\AA}$  Hg  $^1\text{S}_0$ – $^3\text{P}_1$  resonance line) are harmful and must be shielded, together with any surfaces which may reflect that radiation into the surrounding laboratory. Such sources may also stimulate the production of ozone ( $\text{O}_3$ ) which has a characteristic ‘electric’ smell and has well-known corrosive properties on some materials such as rubber.
- 0.2–0.12  $\mu\text{m}$ , 2000–1200  $\text{\AA}$ , 6–10 eV. The vacuum ultra-violet, where atmospheric gases absorb the radiation ( $\text{O}_2$  below 2424  $\text{\AA}$  and  $\text{N}_2$  below 1270  $\text{\AA}$ ), where most materials have lost their transparency and where the reflecting powers of metals are beginning to decline. Optical instruments for this region must be in a vacuum chamber or in a non-absorbing atmosphere such as helium, which is transparent down to 911  $\text{\AA}$ , and other rare gases similarly down to their respective ionisation potentials. It is an interesting and not yet thoroughly explored region where autoionisation series spectra can be detected with their concomitant ‘superallowed’ transitions and broad line absorption spectra. Filling the spectrograph with helium does not ease the vacuum problem so far as leak prevention is concerned but it may ease the stress on thin-film windows.
- 0.12–0.01  $\mu\text{m}$ , 1200–100  $\text{\AA}$ , 10–100 eV. The far- or extreme-vacuum ultra-violet, sometimes called the XUV, where radiation is ionising, where there are no transparent materials except in the form of thin ( $\sim 1$ – $2 \mu\text{m}$ ) films, where reflection coefficients are down to  $\sim 0.1$ – $0.2$  and apart from synchrotron radiation there are no reliable, steady sources of radiation for absorption spectroscopy.

<sup>1</sup> Ultra-Violet-Optical-Infra-Red.

<sup>2</sup> Most optical glasses are opaque below 3500  $\text{\AA}$ .