Refractive Elements in Spectrographs

George W. Hopkins
Analytical/Medical Laboratory
HPL-98-115
June, 1998

E-mail: hopkins@hpl.hp.com

spectrograph, gas monitors, Raman, diffraction grating

A spectrograph design was needed for an application in medical optics. Requirements for resolution were modest, cost was to be minimized, and every photon was precious. The initial design used a concave, aberration-corrected, holographically-recorded, diffraction grating. This design cost too much and collected too few of the precious photons. Several design forms, which use refractive optics with a planar diffraction grating, were investigated. The design that was chosen and built uses two aspheric glass lenses, one for collimating and one for focusing, together with a planar diffraction grating.

To be published in and presented at the *International Optical Design Conference*, 1998, Kona, Hawaii, *Proceedings of the SPIE*, Volume 3482.

Refractive elements in spectrographs

George W. Hopkins

Hewlett-Packard Company
3500 Deer Creek Road
Palo Alto, CA 94304-1392 U.S.A.

Telephone: 650-857-5440
Fax: 650-857-2882
E-mail: hopkins@hpl.hp.com

Abstract

A spectrograph design was needed for an application in medical optics. Requirements for resolution were modest, cost was to be minimized, and every photon was precious. The initial design used a concave, aberration-corrected, holographically-recorded, diffraction grating. This design cost too much and collected too few of the precious photons. Several design forms, which use refractive optics with a planar diffraction grating, were investigated. The design that was chosen and built uses two aspheric glass lenses, one for collimating and one for focusing, together with a planar diffraction grating.

The design task

Our design task was to develop a spectrograph for an operating-room gas monitor based on the Raman effect. This gas monitor is an improvement on a system, developed by Albion (subsequently purchased by Ohmeda), which uses a laser and a build-up cavity to produce an intense light beam that excites gas molecules in a side stream from a patient's airway. A spectrally selective detector measures the Raman emissions, which are very weak, from the metabolic gases and anesthetic agents. Gases can be identified and concentrations determined.

The design is driven by four considerations. Carbon dioxide, which is a prime indicator of a patient's health, needs to be measured with an uncertainty of 0.1 percent or less. The interference between emissions from carbon dioxide and nitrous oxide, which have spectral lines separated by only about 5 nm, must be acceptable. The spectral range must be suitable for identification and measurement of the halogenated anesthetic agents. Finally, cost must be minimized to gain market acceptance.

Specification

Our spectrograph covers the wavelength range from 675 nm to 855 nm. Light from a laser beam, with a waist of 0.106 mm, is imaged onto a planar detector with a linear dispersion of 8.8 mm and a height of 0.608 mm. At least 40 resolution elements across the spectrum are needed. A thin-film filter (the "Rayleigh" filter) blocks the laser light, and a nearly collimated space is needed for this filter. The detection limit is determined by the shot noise in the detection events, so the maximum light collection possible is needed. We used both a small focal ratio for the spectrograph and a windowed tube, concentric with the laser beam and with a reflective coating, to get an adequate signal.

History

Isaac Newton, who discovered that the white light of the sun could be split into colors with a glass prism, made the first observations of spectra in 1666. The first step in spectroscopic instrumentation, the use of two refracting telescopes with a glass prism, followed quickly. One telescope acted as a collimator, with a slit at its focal point. The other telescope, attached to a movable arm, with a goniometer, viewed the light refracted by the prism. This allowed scientists to observe spectral lines and to measure their wavelengths.

The next major practical advance occurred in 1882, when Henry Rowland of Johns Hopkins University produced high quality ruled diffraction gratings. Rowland also invented and produced concave diffraction gratings. He even described the curvature of grooves that would correct aberrations, but he was unable to produce such gratings. Several workers have subsequently developed aberration-corrected, holographically recorded, diffraction gratings, and these are commercially available.

In the years immediately following Rowland's production of planar gratings, several design forms, which used concave mirrors to collimate light and to form images of light diffracted by planar gratings, were developed. These mirror forms allowed spectroscopy in spectral regions where refractive optics did not transmit.

Concurrently, there were advances in detection. The first spectrographs used photographic plates to record spectra. A typical spectrograph, made by Gaertner, used two lenses, called the collimator and camera lenses, together with a prism.

Photoelectric detection was the next major advance. Although W. W. Coblentz built and used a spectrometer with photoelectric detection in about 1900, the earliest commercial spectrophotometer was developed by Arthur Hardy in 1938 and marketed by the General Electric Company. Eventually, photoelectric array detectors, such as the Reticon photo-diode array, became available. The Hewlett-Packard 8450A UV/Visible Spectrophotometer, introduced in 1979, was an early example of an instrument, combining a photo-detector array with a concave diffraction grating, which did not require mechanical scanning.

In more recent times, charge-coupled device (CCD) photo detectors have become available at modest prices, allowing their use in commercial instruments. CCD detectors are very sensitive and can be used in weak-signal applications, such as the measurement of Raman emissions. An instrument designed for this use is the Kaiser Optical Systems f/1.8i VPT SYSTEM, which uses multi-element lenses and collects light at a focal ratio of f/1.8.

The design, which I describe here, is an improvement on spectrometers with CCD detectors, mainly in the area of cost reduction, while maintaining substantial light collecting ability.

Some physics and design limitations

We recommend that designers faced with a task similar to ours familiarize themselves with the first four chapters of Volume V of *Applied Optics and Optical Engineering*, Rudolf Kingslake, Ed., Academic Press (1969). Prisms and diffraction gratings have characteristics, which result in a different approach to design than one would use in designing image-forming optics.

Fundamental to understanding the function of spectrographs is an understanding of the grating equation (Kingslake, p. 21):

$$m\lambda = d(\sin \alpha \pm \sin \beta)$$

α is the angle of incidence, β is the angle of diffraction, d is the groove spacing (period), λ is the wavelength, and m is the diffraction order.

There are two imaging phenomena, which derive from the grating equation. One is grating magnification. When the angle of incidence is equal to the angle of diffraction, a situation called “in Littrow”, the grating magnification is unity. The incident and diffracted beams have the same width. Otherwise, the beam widths differ, and, since the Lagrange invariant is preserved, the grating magnification is not unity. The grating equation also states that there is a non-linear relationship between incident and diffracted rays. If object points are off-axis, as with a straight slit, and the on-axis point is not “in Littrow”, the image of the straight slit is curved. Clearly, a design for which the center of the spectrum is “in Littrow” is advantageous.

Also fundamental to understanding of the function of spectrographs is an understanding of grating efficiency. For gratings with a groove spacing that is comparable to the wavelength of light, grating efficiency must be determined with a theory which accounts for electromagnetic properties of the grating, including both structure and material properties. This theory is complicated. We found efficiency plots in the literature (Loewen, Maystre) to be useful, but we also had such plots for our prospective designs generated by a consultant.

Initial design

Our first prototype spectrograph used a concave, aberration-corrected, holographically recorded, diffraction grating. This design functioned well, but it had several shortcomings. The f/2.3 collection focal ratio was larger than desired. Since the focal ratio at the detector and the detector size determine the Lagrange invariant, this was a fundamental limit. Additional optics, a microscope objective and an achromatic doublet, were required to collect sufficient light and to provide a collimated space for a Rayleigh filter. These added cost. The most serious problem was the potential cost of the diffraction grating in production.

In addition to cost, there were technical problems. Concave gratings with smaller focal ratios than f/2.3 were being offered, but, with a small focal ratio, there are a large spread in angles of incidence on the grating. This makes it difficult to maintain high diffraction efficiency. Cost also increased as the focal ratio decreased.

Literature and patent searches

Due to the importance of intellectual property in our line of work, literature and patent searches were conducted. There is an extensive literature on gratings and spectrographs; reading it can be quite entertaining. Literature that is directly relevant to our design is limited; we recommend (Kingslake, pp. 17-84) and (Datta). The most relevant patents are (Granger) and (Tedesco).

Design software

We employed both OSLO 3 and ZEMAX in our design process. The author was required to use a Hewlett-Packard UNIX workstation (only managers could have PCs in my department, back then). OSLO 3, which is now obsolete, was the only available optical design program, but it was up to the task. The author had a PC at his home, which ran ZEMAX, as did the Hewlett-Packard Division the author was collaborating with. ZEMAX was also suited to the design task.

We found it necessary to write macros to plot images of lines and to estimate spectral line widths at several wavelengths in order to assess performance adequately and to guide our design process. This was done in the OSLO "Star Command" language, and the examples of evaluation of spectrograph performance given later in this paper were produced using OSLO. Kenneth

Moore added a feature to ZEMAX at our request to allow us to trace rays from an extended object, defined by an array of numbers, and determine the fraction transmitted through the system. By representing a detector element as a rectangular aperture, we could perform equivalent evaluations to those done with OSLO 3 star commands.

We found that care must be used in construction of merit functions to guide the design properly. Since aspheric surfaces represented by polynomials were used, the ray grid at the pupil had to be dense enough to sample the effect of aspheric coefficient changes on the image adequately. A rectangular grid was used. Due to the simplicity of the design, it proved best to control only the transverse aberrations in the plane of dispersion. This allowed the images of the slit to lengthen, which caused a loss of energy off of the detector array, but it provided the best resolution. Choosing appropriate weights for transverse aberrations provided this control. We placed zero weight on the transverse aberrations perpendicular to the direction of dispersion, and we chose weightings in the direction of dispersion to give minimum line width, compared to alternative designs, at the 720 nm wavelength, where the carbon dioxide and nitrous oxide lines tend to overlap. Merit function construction was definitely a trial and error process.

Classification of designs

We investigated designs using refractive optics. We explored two basic design forms. One form is in one plane and uses two lenses, one to collimate a beam (the collimator lens) and one to focus the diffracted beams onto the detector (the camera lens). This form can be used with reflection gratings, transmission gratings, and combined diffraction gratings and prisms (which are called grisms). The second form diffracts light out of the plane of incidence. The source and detector are above and below each other, and one lens can be used. Designs with compound lenses with spherical surfaces and designs with single element lenses with aspheric surfaces were optimized and analyzed.

The design hierarchy

As mentioned earlier in "**Some physics** …", the planar grating designs with the best imaging properties, both with respect to grating magnification and aberrations, use the grating in Littrow. This can be achieved with a grism. If a grism were available at costs comparable to a reflective grating, a grism spectrometer would be the preferred design. Such a design can be an in-line design and have excellent performance.

One can obtain similar results with a reflective grating, operating in Littrow, and a single lens. The source, however, is in the middle of the spectrum. In practice, the source is displaced, perpendicular to the direction of dispersion, to provide clearance. This is the out-of-plane design. When this is done, image quality deteriorates. In our application, which includes a thermoelectric cooler for the detector, the needed displacement, even with folding optics, was too great to give satisfactory imagery.

If a transmission grating is used, the physical layout has some additional freedom. Although the spectrograph cannot be in line (a grism is needed for this), smaller angles of diffraction can be used than for reflective gratings (The collimator and camera lenses do not interfere mechanically). Imagery can be better than for a spectrograph with a reflective grating.

A spectrograph with a reflective grating is at the bottom of the design hierarchy in terms of image quality. This is due to the need for adequate angles of diffraction to avoid physical interference of the collimator and camera lenses, which places the central diffracted ray far off Littrow. The result is varying grating magnification, greater than unity, which is a major contributing factor to spreading of images. But the design is at the top of the (low) cost hierarchy, and it is adequate, making it our preferred form.

Multi-element spherical lenses, up to three elements per group, were inferior to the aspheric lenses in image quality and offered no significant cost advantage.

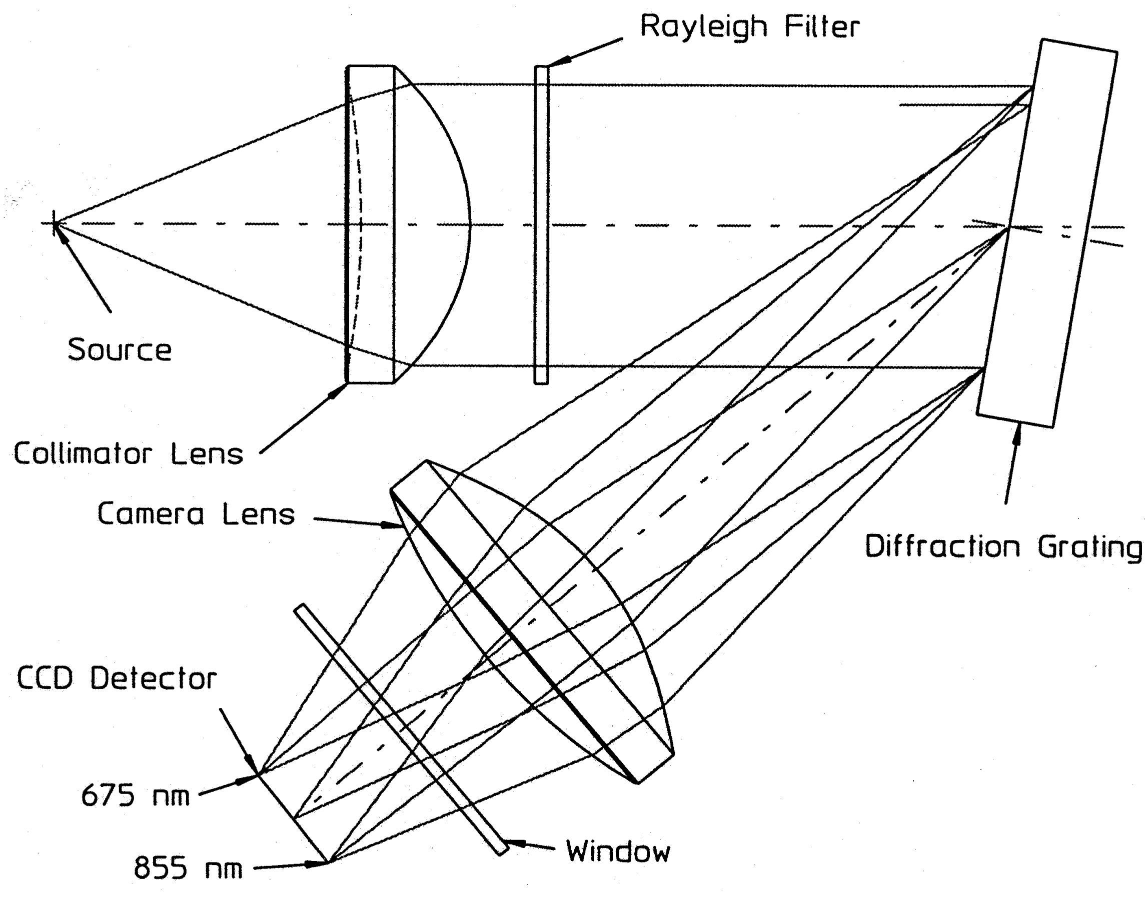
Cost considerations

There is a substantial difference in the cost of manufacturing different designs. Since our goal was minimum cost, consistent with meeting specifications, cost was the main driver. The cost of a critical component, the grating, ranged over a factor of five, from the least to the most expensive: planar reflective, planar transmission, grism and holographically-recorded concave grating.

All designs require additional optics. The additional optics for the concave grating are a relay, with a collimated space for a Rayleigh filter. With this design, a slit can be used. The designs with the planar gratings, including the grism, require only a collimating and a camera lens. The optics for these designs was similar in cost, which was less than the cost of the additional optics for the concave grating.

The preferred design

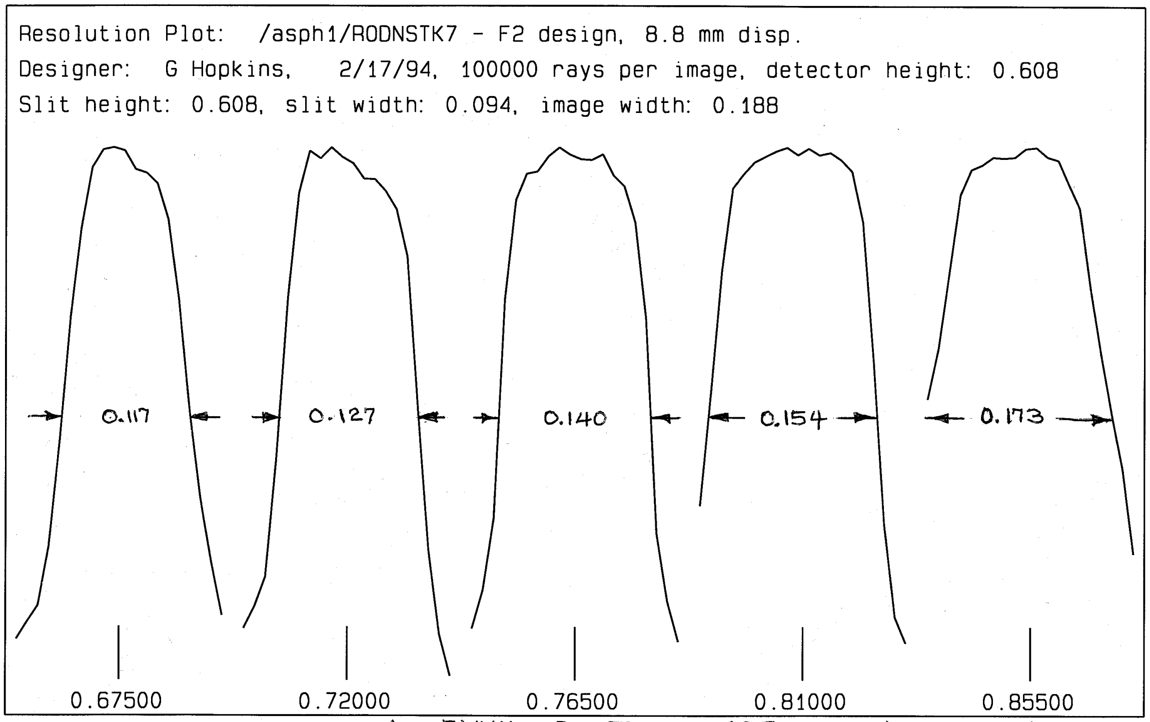
The design selected for our prototype spectrograph was an in-plane design with two, single-element, aspheric lenses. These are formed of F2 glass. A 1200 line-pair-per-mm, planar, diffraction grating, blazed for 750 nm, is used. The design and design methodology are described in detail in U. S. Patent 5,644,396 (Hopkins), so the detail is not reproduced here.



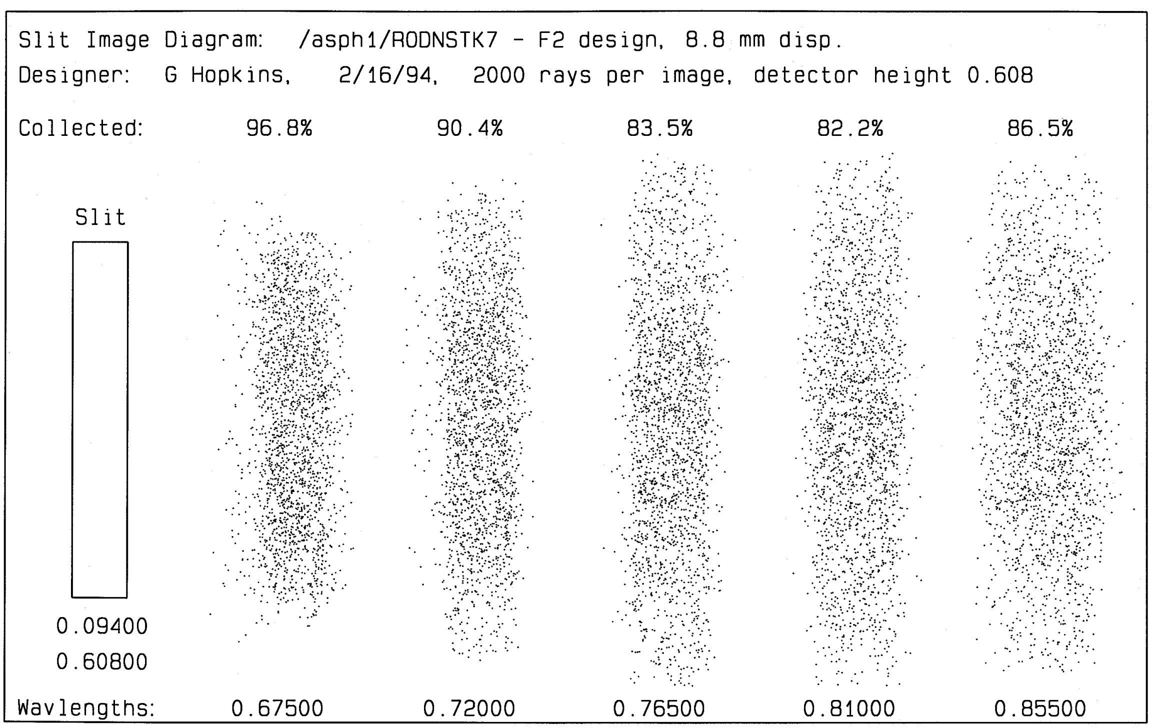
The lenses are formed by molding. F2 glass was chosen, in combination with an invar support structure, to improve stability of image position and focus with temperature changes.

The detector array is tilted slightly with respect to the axis of the camera lens to give first-order compensation for axial chromatic aberration.

The figures on the following page indicate the imagery achieved with the design. Note the effects of grating magnification on line width and height.



Represents W_0 = 0.080 mm, Avg. FWHM = 0.145 mm, 60.7 resolution elements.



Five prototype spectrographs (Bach, Beethoven, Brahms, Barber and Bernstein) were fabricated to this design and tested. These spectrographs performed according to predictions.

Acknowledgements

The author is grateful for the following contributions to the spectrograph development. Tad D. Simons designed the original concave grating spectrograph and assisted the author throughout the project. Peter Ast handled vendor negotiations, obtained the aspheric lenses and took part in testing the completed spectrographs. Michel Neviére, of the Faculté des Sciences et Techniques, Centre de Saint-Jérôme, Marseille, France, computed diffraction grating efficiencies for several prospective designs. Rick Pittaro, my project manager, was an unrelenting advocate of collecting that last precious photon. My employer, Hewlett-Packard Company, provided an outstanding work environment, the time needed to study this design problem thoroughly, and the opportunity to present my work here at the International Optical Design Conference on the Big Island of Hawaii.

References

Carlsen et al. 1995 - U. S. Patent 5,450,193, *Raman spectroscopy of airway gases*.

Carlsen et al. 1996 - U. S. Patent 5,505,678, *System for collecting weakly scattered electromagnetic radiation*.

Datta - Sunil K. Datta, A Simple Low-Cost Grating Spectrograph for the Optical Region (350-700 nm), *Indian Journal of Pure & Applied Physics*, Vol. 22, November 1984, pp. 667-669.

Granger - U. S. Patent 4,895,445, *Spectrophotometer*.

Hopkins, II - U. S. Patent 5,644,396, *Spectrograph with low focal ratio*.

Kingslake, Ed., *Applied Optics and Optical Engineering*, Volume V, Chapters 1-4, Academic Press (1969).

Loewen – E. G. Loewen, M. Neviére and D. Maystre, "Grating efficiency theory as it applies to blazed and holographic gratings", *Applied Optics*, Vol. 16, No. 10, pp. 2711-2721, October 1977.

Maystre – D. Maystre, M. Neviére, and R. Petit, "Experimental Verifications and Applications of the Theory", *Electromagnetic Theory of Gratings*, R. Petit, Ed., Electromagnetic Theory of Gratings, Springer-Verlag, 1980.

Tedesco et al. – U. S. Patent 5,011,284, *Detection system for Raman scattering employing holographic diffraction*.