Diffraction Gratings

"It is difficult to point to another single device that has brought more important experimental information to every field of science than the diffraction grating." - George Harrison
Diffraction Grating History

- First constructed by David Rittenhouse, but not applied (1785).
- Interested Fraunhofer as a tool for spectroscopy. It was via gratings that he observed spectral absorption lines in the Sun (1821)
- "Commercial" production began in Prussia and U.S. (1850-1870)
- Development of precise ruling engines (1900)
- True commercial production of precision diffraction gratings (1950)
Create parallel groves which enforce a phase lag with each adjacent reflection.

Grooves can be transparent/opaque rulings on a transmissive material, formed by opaque lines on a mirror, or consist of tilted facets.

Phase lags with integral multiples of a given wavelength interfere constructively.
Diffraction Gratings

- Light of a given wavelength interferes constructively if

\[ d(\sin \alpha + \sin \beta) = m\lambda \]

where \( m \) is an integer

note the sign convention for the angles involved

\[ \text{Figure 2-2. Geometry of diffraction, for planar wavefronts. The terms in the path difference, } d \sin \alpha \text{ and } d \sin \beta, \text{ are shown.} \quad \text{Diffraction Grating Handbook (RGL)} \]
For normal incidence, $\alpha=0$,

$$d\sin \beta = m\lambda \quad \lambda(\beta) = \frac{d\sin(\beta)}{m}$$

• a given direction transmits a variety of wavelengths related by integral fractional multiples.

• a given wavelength can appear in many directions
Grating Dispersion

\[ \lambda = \frac{d \sin \beta}{m} \quad \frac{d \beta}{d \lambda} = \frac{m}{d \cos(\beta)} \]

- Angular dispersion increases with
  - decreasing groove spacing
  - increasing order

- Spectral resolution, however, depends only on the angle off of the grating.
  - low resolution: normal incidence and reflection
  - high resolution: reflection (and often incidence) well off grating normal

\[ R = \frac{\lambda}{\Delta \lambda} = \tan(\beta) \frac{1}{\Delta \beta} \]

for normal incidence
Grating Spectrograph Configurations

- Since spectrographs are simply imagers, they suffer from all of the aberrations endemic to optical systems.
- Spectrograph configurations seek to minimize aberrations and maximize grating efficiency.
  - Small angular deviation generally yields good efficiency.

- **Littrow configuration**
  - minimizes the angular deviation
  - maximizes efficiency

- **Czerny-Turner**
  - a close relative is the Ebert-Fastie which uses a monolithic mirror.
Littrow Configuration

\[ d(\sin \alpha + \sin \beta) = m\lambda \quad \alpha = \beta \]

\[ \lambda = \frac{2d \sin \beta}{m} \]

- Littrow
  - minimizes the angular deviation
  - maximizes efficiency
  - enforces compact design

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Figure 6-4. The Littrow monochromator mount. The entrance and exit slits are slightly above and below the dispersion plane, respectively; they are shown separated for clarity.
Grating Spectral Response and Resolution

- Explain this...

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**Figure 5.1.** The function $I(u)$. The function itself is the solid line and the factor $\text{sinc}^2 u$ which envelopes the function is shown as a broken line. In this drawing the constant $k$ has been chosen equal to 3, so that the 3rd, 6th, 9th etc. orders are suppressed.
Grating Performance and the Convolution Theorem

\[ f(x)g(x) = F(\nu) * G(\nu) \quad \text{and} \quad f(x) * g(x) = F(\nu)G(\nu) \]

What does this have to do with gratings?

- The far-field response to a plane wavefront reflecting off (or passing through) an aperture is the Fourier Transform of the reflected wavefront.

- A grating is an aperture which modifies a plane wave. The emerging wavefront can be considered the product/convolution of three functions.
  - a single grating facet
  - convolved with a picket fence of delta functions
  - multiplied by the aperture of the grating

\[ \text{grating} = \text{aperture} \times (\text{groove} \times \text{picket fence}) \]

Each has a well defined Fourier transform

\[ \text{angular response} = \text{aperture}(\theta) \times (\text{groove}(\theta) \times \text{picket_fence}(\theta)) \]
Grating Performance and the Convolution Theorem

\[ f(x)g(x) = F(\nu) * G(\nu) \]

\[ f(x) * g(x) = F(\nu)G(\nu) \]

- The Fourier Transform of a square aperture is a sinc function (e.g. single slit diffraction).
  - The individual groove produces a broad sinc function in the Fourier domain since it is spatially narrow – it multiplies the entire response.
- The Fourier Transform of a picket fence is a picket fence of spatial frequency proportional to \( \frac{1}{d} \)
- A infinite grating is a convolution of a picket fence with single slits. The response is an infinite series of angular peaks modulated by the sinc function of the single slit.

![Grating Design](image.png)

**Figure 5.1** The function \( f(\omega) \). The function itself is the solid line and the factor \( \text{sinc}^2 \omega \) which envelopes the function is shown as a broken line. In this drawing the constant \( k \) has been chosen equal to 3, so that the 3rd, 6th, 9th etc. orders are suppressed.
Grating Performance and the Convolution Theorem

\[ f(x)g(x) = F(\nu) * G(\nu) \]

\[ f(x) * g(x) = F(\nu) G(\nu) \]

• Finally, the aperture of the full grating is a product of a square aperture function with the picket fence.

• In Fourier space this is a convolution of the full aperture sinc function (a skinny one representing diffraction of the full aperture) with the infinite picket fence of monochromatic peaks.

\[ I(\theta) = I_o \left| \sin \frac{\beta}{\beta} \right|^2 \left| \frac{\sin N \gamma}{N \sin \gamma} \right|^2 \]

\[ \beta = \frac{\pi}{\lambda} w \sin \theta \quad \text{w is the width of a reflective facet} \]

\[ \gamma = \frac{\pi}{\lambda} d \sin \theta \quad \text{d is the groove spacing ( w < d )} \]

Figure 5.1. The function \( I(u) \). The function itself is the solid line and the factor \( \text{sinc}^2 u \) which envelopes the function is shown as a broken line. In this drawing the constant \( k \) has been chosen equal to 3, so that the 3rd, 6th, 9th etc. orders are suppressed.
Diffraction Limited Grating Resolving Power

- The angular width of a diffraction peak is limited by the physical size, $W$, of the grating (seen tilted in projection at the diffracted angle).
  \[ \Delta \theta = \frac{\lambda}{W \cos \beta} \]

- The grating size can be expressed in terms of the number of grooves, $N$, and their spacing $d$.
  \[ \Delta \theta = \frac{\lambda}{Nd \cos \beta} \]

- Recalling
  \[ \lambda = \frac{d \sin \beta}{m} \quad \frac{d \beta}{d \lambda} = \frac{m}{d \cos(\beta)} \]

- Resolution depends on only the total number of grooves and the spectral order
  \[ R = \frac{\lambda}{\Delta \lambda} = \frac{\lambda}{\frac{d \lambda}{d \beta} \Delta \theta} = mN \]
Grating Performance – Blaze and Efficiency

- Grating facets are tilted (the phase of the reflection is tuned) to concentrate the Fourier maximum of the single facet sinc function in a desired direction/wavelength.
  - Echelle configuration (high angle = high resolution) being an extreme case.
- Ideally the blaze angle equals the incident/emergent angle for Littrow operation.
  - In practice the angular deviation is non-zero to accommodate optics.

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**Figure 11-3.** Echelle geometry. The groove spacing $d$, step width $t$ and step height $s$ are shown. GN is the grating normal and FN is the facet normal. The blaze arrow (shown) points from GN to FN.
Grating facets are tilted (the phase of the reflection is tuned) to concentrate the Fourier maximum of the single facet sinc function in a desired direction/wavelength.

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The Diffraction Grating Handbook (RGL)

*Figure 9-1. A typical (simplified) efficiency curve.* This curve shows the efficiency $E$ of a grating in a given spectral order $m$, measured vs. the diffracted wavelength $\lambda$. The peak efficiency $E_p$ occurs at the blaze wavelength $\lambda_B$. 

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Grating Efficiency

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Grating Efficiency

Figure 5.4. Relative efficiency of a diffraction grating as a function of wavelength.

(a) Blaze angle = 20°. Wavelength scale for a grating of 6000 lines/cm.
(b) Blaze angle = 40°. Wavelength scale for a grating of 6000 lines/cm.

Design of Optical Spectrometers (James and Sternberg)
Gratings and Polarization Effects

Figure 9-2. *S* and *P* polarizations. The *P* polarization components of the incident and diffracted beams are polarized parallel to the grating grooves; the *S* components are polarized perpendicular to the *P* components. Both the *S* and *P* components are perpendicular to the propagation directions.

Figure 9-7. Same as Figure 9-5, except 14° blaze angle. The curve for unpolarized light (marked U) is also shown; it lies exactly halfway between the *S* and *P* curves.

Figure 9-8. Same as Figure 9-5, except 19° blaze angle.
Grisms

- A grating can be applied to a transparent substrate such that prism refraction and grating diffraction can be combined. Such a configuration can provide
  - order separation (cross dispersion)
  - linearization of dispersion
  - zero deviation angle

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*Figure 11-2. Grating prism (grism).* Ray path for straight-through operation at one wavelength.
Holographic Gratings

In addition to mechanical ruling, gratings can be created by casting interference fringes on a photographic medium.

Ironically, ruled gratings can be manufactured with finer groove spacing than holographic gratings.

Holographic gratings do not suffer from periodic ruling errors. As a result, they tend to be more ghost free.

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**Figure 4-3.** First-generation recording method. Laser light focused through pinholes at A and B diverges toward the grating blank (substrate). The standing wave region is shaded; the intensity maxima are confocal hyperboloids.

**Figure 4-4.** Groove profiles for ruled and holographic gratings. (a) Triangular groove profile of a mechanically ruled grating. (b) Sinusoidal groove profile of a holographic grating.
Replica Gratings

- Generating a grating directly on a glass or metallic substrate is an expensive and time consuming process.
  - Commercial gratings of modest cost are produced by replicating a “master” ruling in epoxy.
  - After creating the replicated epoxy layer a reflective coating (gold or aluminum) is applied to the epoxy.
  - The grating store tends to sell only a limited range of offerings based on the stock of master rulings.

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*Figure 5-1. The replication “sandwich”, showing the substrates, the epoxy layers, metallic coatings, and the parting agent.*
Ruling Engines

- A ruling engine must cut a cleanly shaped groove free of periodic errors and other distortions – otherwise ghosts will contaminate the spectrum.
Although they are of a completely different nature, Fabry-Perots are like gratings in the sense that they stack up successive phase delays between wavefronts to produce constructive and destructive interference.

Instead of using multiple spatially-separated phase centers to produce the delay, the Fabry-Perot uses multiple reflections between a pair of highly reflective (and most importantly weakly transmissive) surfaces.

The anti-reflection coating is a low-quality (intentionally) Fabry-Perot cavity.
Fabry-Perots are like gratings in the sense that they stack up successive phase delays between wavefronts to produce constructive and destructive interference.

Instead of using multiple spatially-separated phase centers to produce the delay, the Fabry-Perot uses multiple reflections.
The separation between mirrors determines the order of interference and thus the free spectral range (wavelength spacing between peaks).

Constructive interference is obtained if the path length difference between the mirrors \((2d)\) is an integral number of wavelengths.

Usually the cavity is 1000s of wavelengths wide. The FSR might be the difference between transmission in order 5072 and 5073

\[
FSR = \frac{\lambda_m - \lambda_{m-1}}{m} = \frac{2d}{m} - \frac{2d}{m-1} \approx \frac{2d}{m^2} = \frac{\lambda^2}{2d}
\]

The surface reflectivity determines the spectral sharpness of the transmission peaks and thus is a factor in determining spectral resolution (finesse).

\[
\Delta \lambda = \frac{FSR}{Finesse}
\]

\[
\lambda = \frac{2d}{m \cos(\theta)}
\]
Pratical Fabry-Perots

- Fabry-Perot Interferometers are traditionally high spectral resolution devices because they can be operated at very high order m.
  - To achieve $R=100,000$ at $1.0\mu m$, given a finesse of 40 ($r=0.96$)...
    - $m=2500$ and $d=2500\mu m$ or 2.5mm
- The reflective Fabry Perot plates are the key to good performance.
  - To achieve good resolution plate reflectivity must be quite high (95% or greater).
  - Plates must be plane parallel to arcseconds
  - Fabry Perots are basically monochromatic filters. Plates must be tuned in separation in order to scan in wavelength (maintaining parallelism).
    - Unwanted adjacent orders – just one free spectral range away – must be filtered out (often using a second “tandem” Fabry Perot cavity.)
Fabry Perot Implementations

- Plate separations are tuned by
  - micrometers
  - piezoelectric crystal stacks
  - varying the pressure (and thus refractive index) in the gaps between the plates
- In all cases, the plate separation must be scanned by half of a wavelength in order to scan a transmission peak across the free spectral range
Fabry-Perots must be scanned in wavelength to obtain a spectrum.
Since Fabry-Perots are simply extremely narrowband filters, spectra are collected in "image cubes" one monochromatic image at a time.
Reduction is complicated by the fact that wavelength transmission varies with angle (image slices are bowed in wavelength).
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Fabry Perot Image Cubes

http://www.sao.ru/hq/moisav/scorpio/ifp/cubes.html