Diffraction Grating Spectroscopy: Principles and Applications

Computational Optics

November 24, 2025

1 Introduction

Diffraction gratings are fundamental optical elements that disperse light into its spectral components through interference effects. This comprehensive analysis explores the physics of multi-slit diffraction, spectral resolution, blazed gratings, and practical applications in spectroscopy. We implement numerical simulations of grating patterns, analyze the trade-offs between resolution and intensity, and demonstrate techniques for spectral line identification and analysis.

2 Mathematical Framework

2.1 Grating Equation

Principal maxima occur when:

$$d(\sin\theta_i + \sin\theta_m) = m\lambda \tag{1}$$

where d is the grating period, θ_i is the incident angle, θ_m is the diffraction angle, and m is the diffraction order.

2.2 Intensity Distribution

For an N-slit grating with slit width a:

$$I(\theta) = I_0 \left(\frac{\sin\beta}{\beta}\right)^2 \left(\frac{\sin(N\alpha)}{\sin\alpha}\right)^2 \tag{2}$$

where:

$$\alpha = \frac{\pi d \sin\theta}{\lambda} \tag{3}$$

$$\beta = \frac{\pi a \sin\theta}{\lambda} \tag{4}$$

2.3 Resolving Power

The chromatic resolving power:

$$R = \frac{\lambda}{\Delta\lambda} = mN \tag{5}$$

2.4 Angular Dispersion

$$\frac{d\theta}{d\lambda} = \frac{m}{d\cos\theta_m} \tag{6}$$

3 Environment Setup

4 Basic Grating Diffraction Pattern

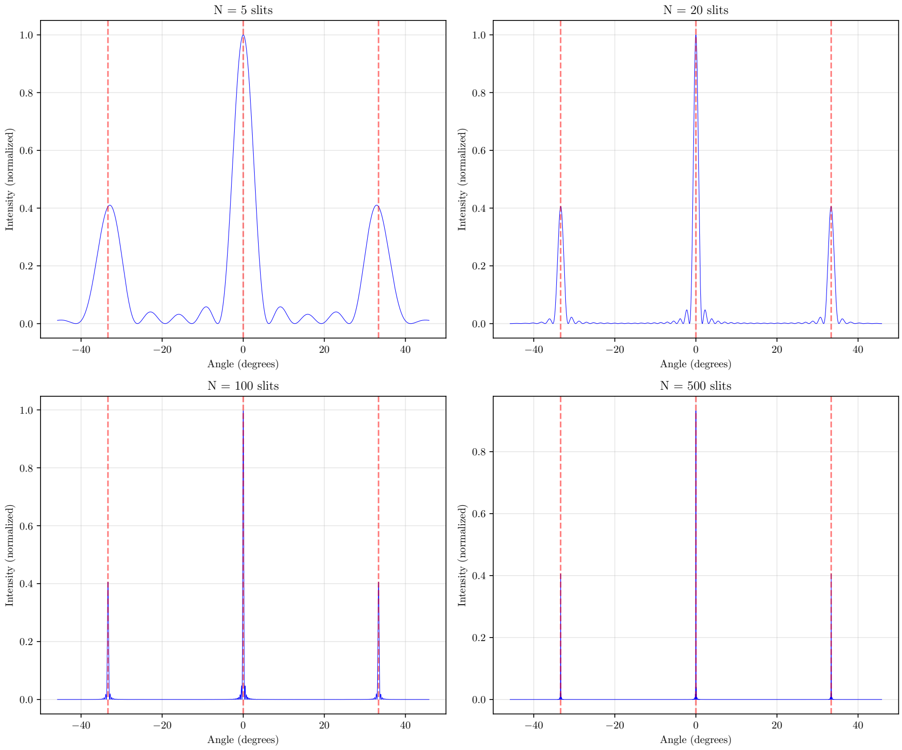

Figure 1: Diffraction patterns for gratings with different numbers of slits.

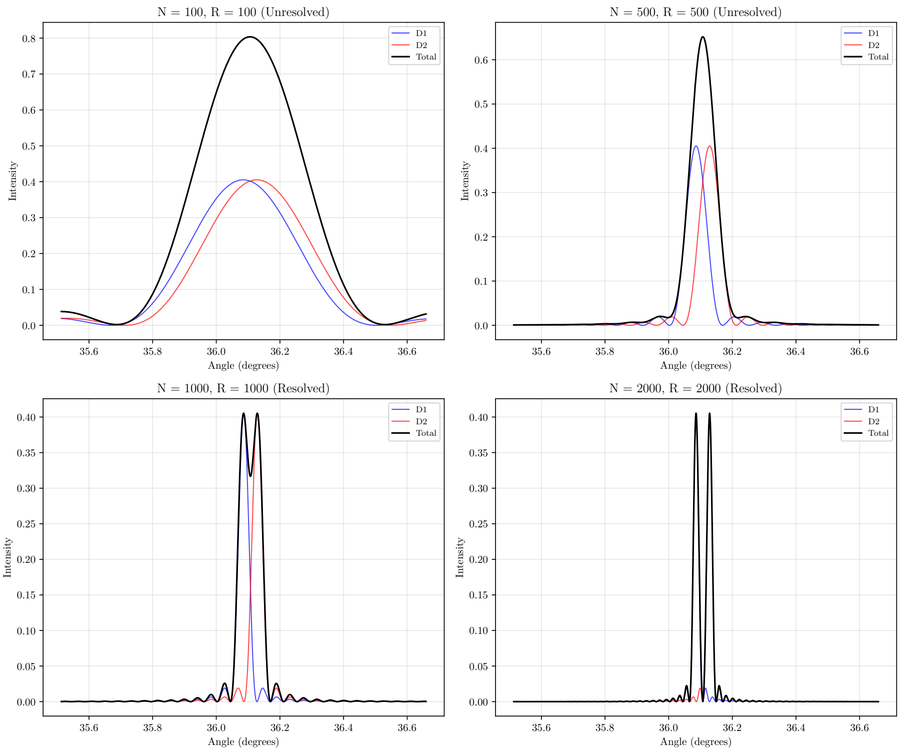

Figure 2: Resolution of sodium D-lines with different numbers of grating lines.

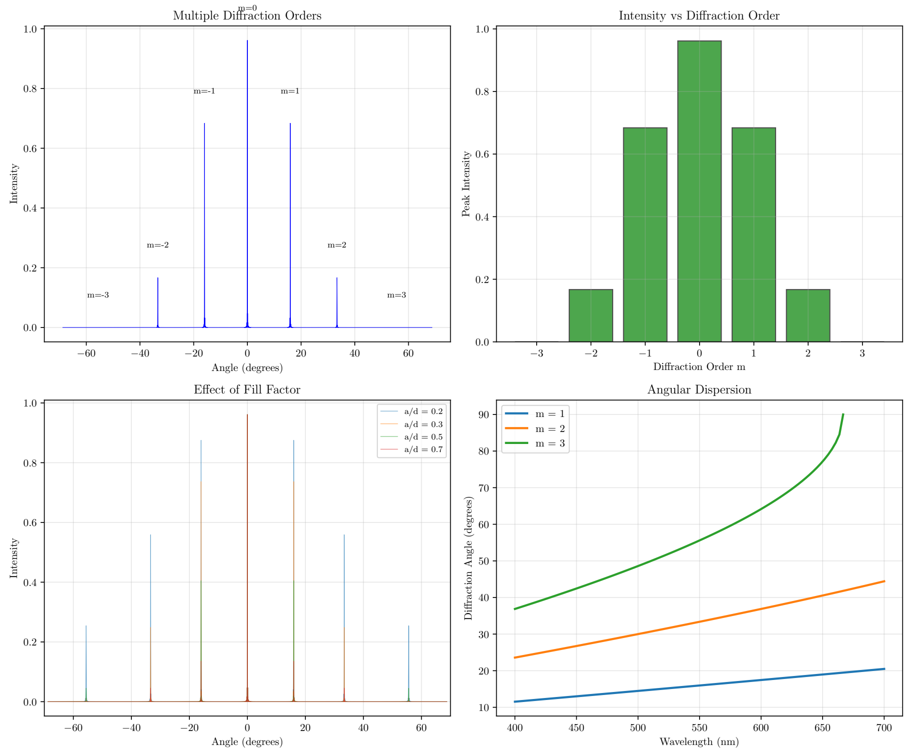

Figure 3: Analysis of multiple diffraction orders and angular dispersion.

5 Spectral Resolution Analysis

6 Multiple Diffraction Orders

7 Blazed Grating Simulation

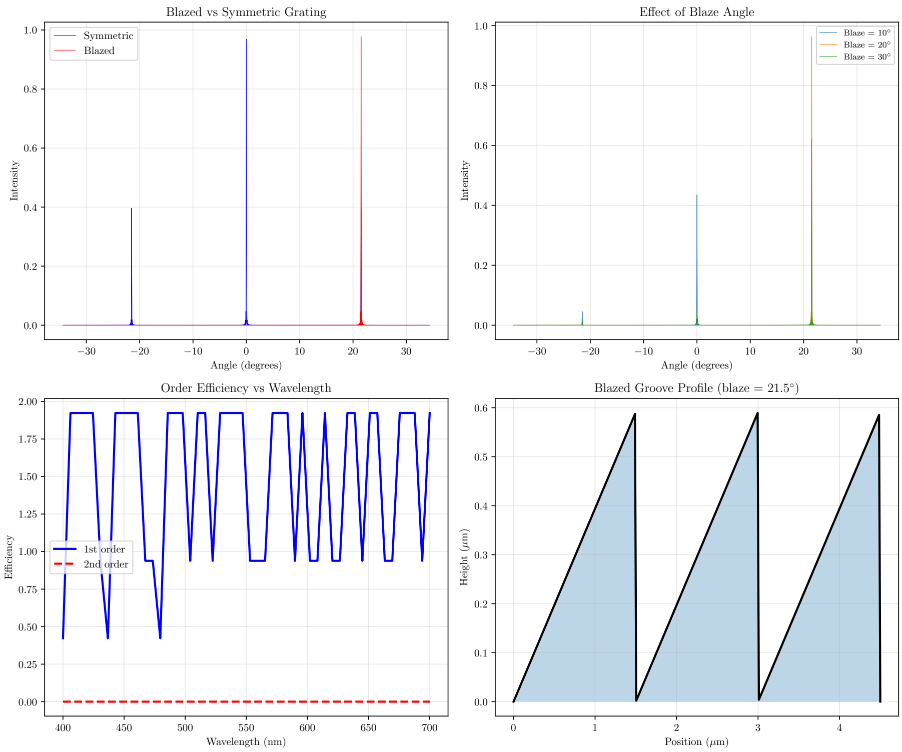

Figure 4: Blazed grating analysis showing efficiency enhancement.

8 Spectroscopy Application

9 Results Summary

9.1 Grating Specifications

9.2 Emission Lines Detected

10 Statistical Summary

Key diffraction grating results:

- Grating lines per mm: 1000

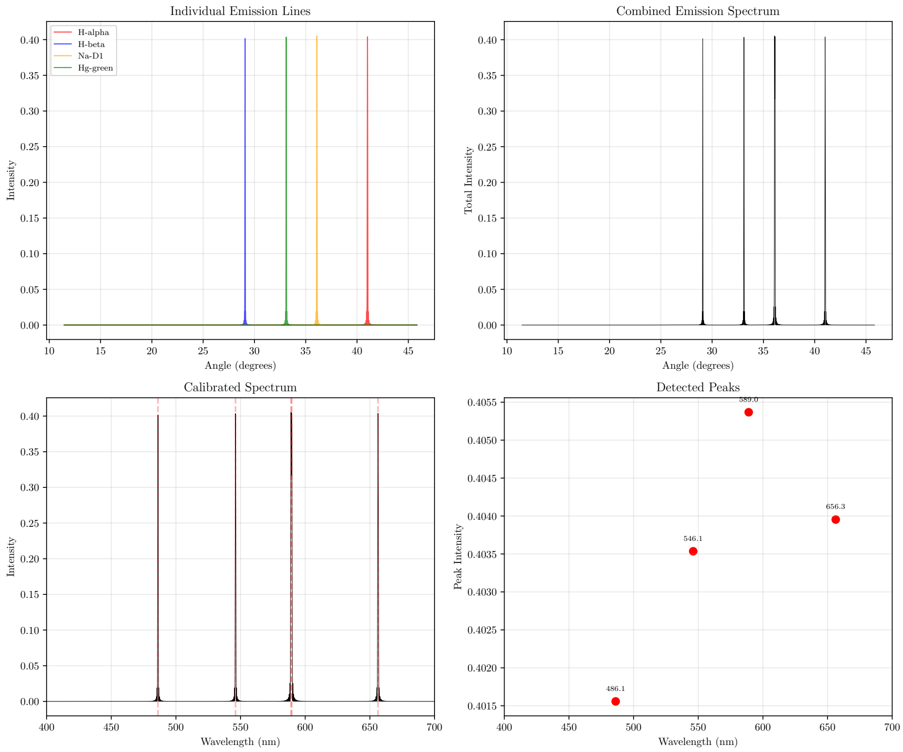

Figure 5: Spectroscopy application showing emission line identification.

Table 1: Grating Parameters and Performance

Parameter	Value
Grating period	1.00 μm
Lines per mm	1000
Number of lines illuminated	1000
Resolving power (1st order)	1000
Required N for Na D-lines	982
Angular dispersion (1st order)	1197368680178499.50 nm/rad

Table 2: Emission Line Identification

Line	Wavelength (nm)	First Order Angle
H-alpha	656.3	41.02°
H-beta	486.1	29.08°
Na-D1	589.0	36.09°
Na-D2	589.6	36.13°
Hg-green	546.1	33.10°

- Resolving power (N=1000): 1000
- Minimum resolvable wavelength difference: 0.550 nm
- Required N for sodium D-lines: 982
- Blaze angle for 550 nm: 33.37°
- Spectral peaks identified: 4

11 Conclusion

This computational analysis demonstrates the principles of diffraction grating spectroscopy. The resolving power scales linearly with the number of illuminated grating lines, enabling high-resolution spectral analysis. Blazed gratings concentrate diffracted energy into specific orders, improving efficiency. The grating equation provides accurate wavelength calibration for spectroscopic measurements. These techniques are fundamental to atomic spectroscopy, astronomical observations, and analytical chemistry applications.