Performance Comparison of Spectrometers Featuring On-Axis and Off-Axis Grating Rotation

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Introduction

The majority of modern spectrographs and scanning monochromators produced today feature computer controlled direct digital scanning mechanisms rather than sine bar assemblies for grating rotation. The basic optical arrangement is shown in Figure 1. These direct digital systems incorporate microstepping motors to allow for accurate and reproducible wavelength selection as well as high speed wavelength scanning. Turrets are easily accommodated for multiple gratings, providing expanded spectral coverage and/or variable dispersion if desired.

Prior to the development of direct digital scanning systems, sine drive systems clearly dominated the small monochromator market. In traditional sine drive designs the axis of grating rotation is placed at the face of the grating. In direct digital systems the axis of rotation may be at the face of the grating or on the central axis of the turret, as shown in Figure 2. In this discussion, spectrometers that rotate a grating about its face will be referred to as “on-axis” and those that rotate the grating about the turret axis will be referred to as “off-axis”. Manufacturers of both methods of grating rotations have made claims as to performance superiority. Issues of spectral resolution, focal plane flatness, astigmatism, and overall throughput have been raised. One manufacturer was issued a U.S. patent for an off-axis design, which claims superior line shape and focal plane flatness. Acton Research Corporation (ARC) has been manufacturing spectrometers with on-axis rotation since 1979 and state-of-the-art direct digital spectrometers with off-axis rotation since 1989. We have several thousand off-axis working units in the field with focal lengths that vary from 0.15m to 0.75m. ARC chose the off-axis design because ray trace analysis showed a bias toward better performance. The off-axis design is also mechanically robust and easier to produce. In order to evaluate the conflicting claims, ARC manufactured and tested spectrometers featuring both designs.

Evaluation Systems:
ARC manufactured two 300mm imaging spectrometers employing toroidal mirrors, one with on-axis grating rotation and one with off-axis rotation. Both instruments used standard optical components taken from stock. Aside from the point of rotation, the optical geometries were identical. Both instruments were manufactured to ARC’s published specifications, and each was equipped with a 1200g/mm grating. All tests were conducted with full f/4 illumination.

Performance Comparison in Monochromator Configuration:
The key performance issues when spectrometers are used in a monochromator configuration are spectral resolution and throughput. The only aspect of an off-axis design that could affect throughput would be the potential underfilling of the grating as it translates away from the collimating mirror and potential overfilling of the focusing mirror. By using sufficiently large optics in the ARC off-axis design, the grating remains fully illuminated throughout the entire scanning range and the focusing mirror collects all of the available light, thus throughput is maximized (See Figure 3).

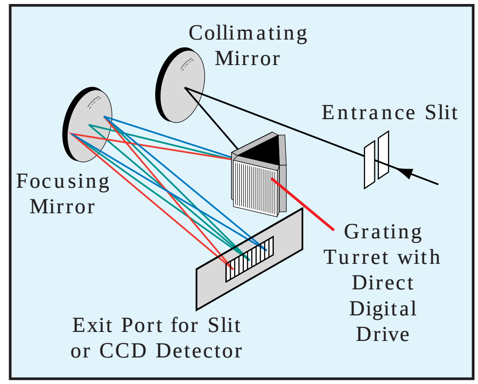


Figure 1: Spectrometer Optical System

Spectral Resolution as a Scanning Monochromator:
The entrance and exit slits of the monochromators were set to 10µm wide by 4mm high and a PMT was placed at the exit. The spectrum of the 435.8nm mercury (Hg) line was scanned and measured for FWHM (full width at half maximum intensity). The off-axis instrument achieved 0.089nm FWHM while the on-axis instrument achieved 0.099nm FWHM. Representative curves are shown in Figure 4. The off-axis system in this case achieved 11% better spectral resolution, however as both instruments fell within normal manufacturing tolerances (typically between 0.07nm and 0.10nm), we conclude that both designs provide acceptable spectral resolution.

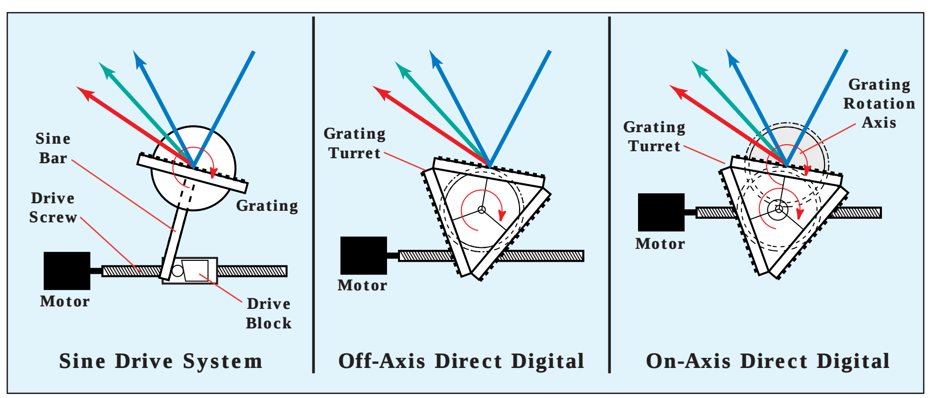


Figure 2:
Left: Conventional sine drive scanning system with precision drive screw, drive block, and sine bar. The motor turns the drive screw which moves the drive block which in turn pushes the sine bar to rotate the grating.

Middle: Direct digital scanning system with worm/worm gear arrangement. The stepping motor turns the worm gear mechanism which rotates the grating turret a full 360°, allowing for wavelength scanning and grating changes.

Right: Direct digital scanning system that rotates the grating about its face (on-axis). A motor turns the worm gear to change wavelengths. A second motor or complex mechanical arrangement changes the gratings.

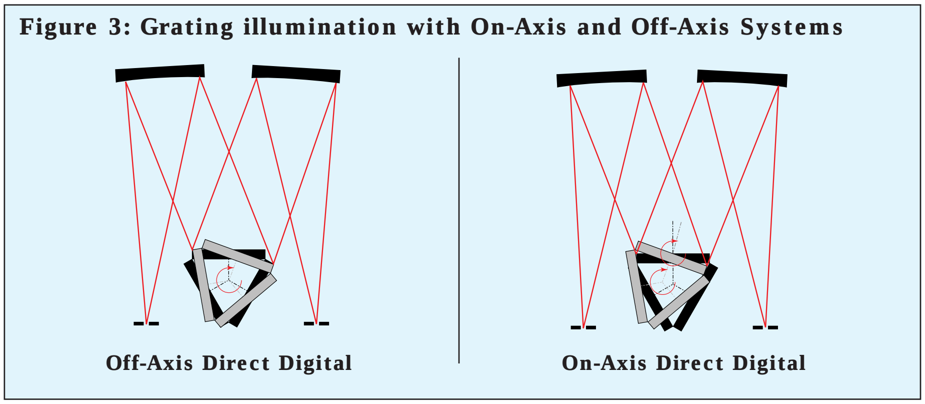
Illumination Issues:
A monochromator can be used as an illuminator, such that the output from the exit slit illuminates a sample or is reimaged on to a sample. For the on-axis and off-axis monochromators used in this evaluation, all rays over the full scanning range of the gratings are contained within the original f/4 cone of light. Therefore sample illumination is equal for both systems.

Performance Comparison in Spectrographic Mode:
The major criteria for evaluation of a spectrograph are focal plane flatness and astigmatism. The degree to which the focal plane is curved or tilted will affect the focus across a planar detector such as a CCD. If the field is sufficiently curved or tilted then the spectral resolution across the detector will degrade with displacement from the central axis.

Astigmatism:
Astigmatism is a normal geometric optical aberration caused by the use of spherical mirrors at off-axis angles. It occurs because spherical mirrors used off-axis form two focal planes, tangential and sagittal as illustrated in Figure 5. Placing the detector in the tangential focal plane will eliminate horizontal astigmatism at the expense of spatial image quality. Placing the detector in the sagittal focal plane will conversely eliminate vertical astigmatism at the expense of spectral resolution. As spectral information is always more important in traditional spectroscopic applications, detectors are usually placed in the tangential focal plane. This causes a point light source to become vertical line images as light passes through a conventional spectrograph or monochromator, as illustrated in Figure 6. Large area single channel detectors such as photomultiplier tubes, photographic plates, and linear focal plane arrays are capable of collecting the entire image, even if the image is several millimeters high. Thus the issue of vertical astigmatism is not of major consequence for conventional spectrometers using these specific detectors.

Importance of Imaging Spectrographs for CCD Detectors:
Today most spectrographic measurements are made with matrixed solid state focal plane arrays such as CCDs. CCD detectors allow the user to capture multiple spectra simultaneously by reading out grouped rows of pixels as separate spectra. Several fiberoptic cables vertically aligned at the entrance slit

Figure 3: Grating illumination with On-Axis and Off-Axis Systems



Left: Off-Axis Grating Rotation: Multiple gratings are mounted on a turret which rotates about its central axis. **ARC's optical system is set up to fully illuminate each grating throughout its entire scanning range, thus throughput is maximized.** This simple and rugged drive arrangement allows for both wavelength scanning and grating changes with a single motor/gear arrangement.

Right: On-Axis Grating Rotation: Multiple gratings are mounted on a turret which rotates about the face of the gratings for wavelength scanning and then about the turret axis for grating changes. This normally requires a second motor, or a more complex mechanical arrangement, adding to potential long term stability issues.

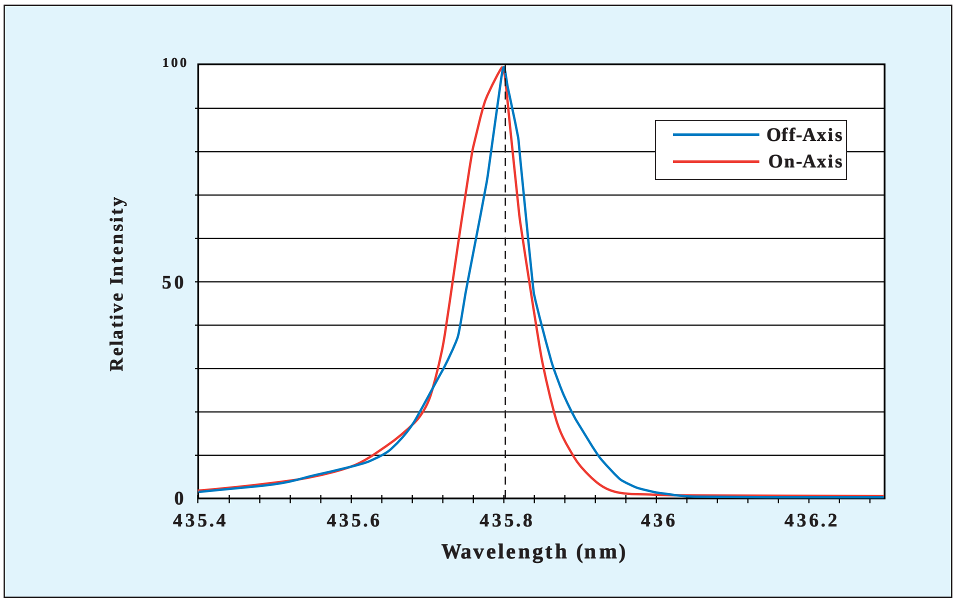
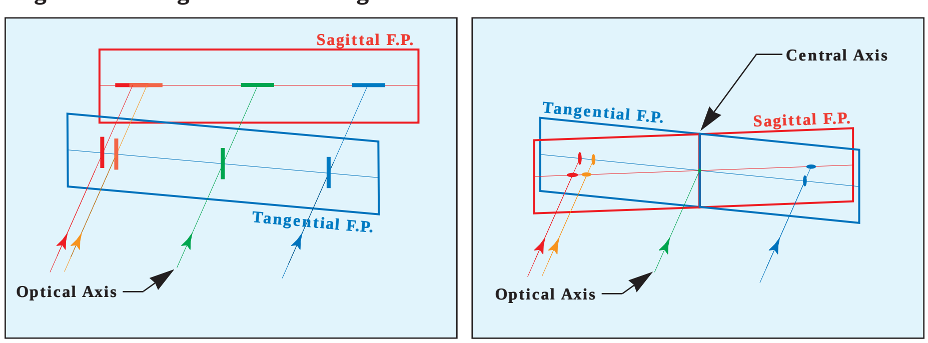


Figure 4: Spectra lines produced by on-axis and off-axis scanning monochromators

Figure 5: Tangential and Sagittal Focal Planes



Tangential and sagittal focal planes formed by the use of spherical mirrors at off-axis angles. A detector on the tangential focal plane detects sharp vertical lines for best spectral resolution.

Tangential and sagittal focal planes are brought together by toroidal mirrors. Images on the tangential focal plane are reasonable stigmatic, preserving spectral and spatial information about the light source.

Figure 6: Astigmatism in Conventional Spectrometers Systems

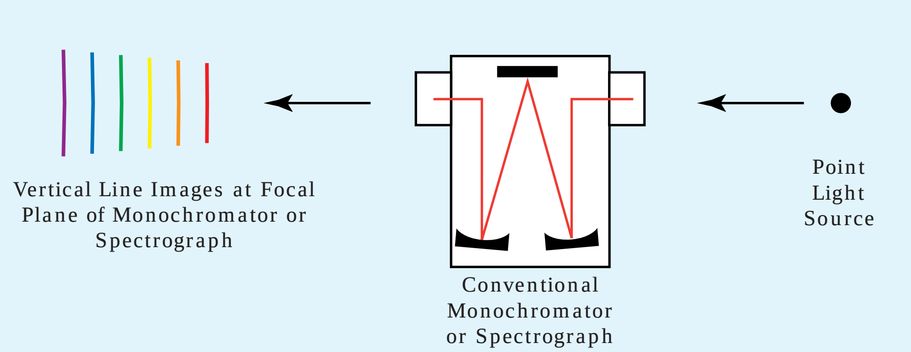
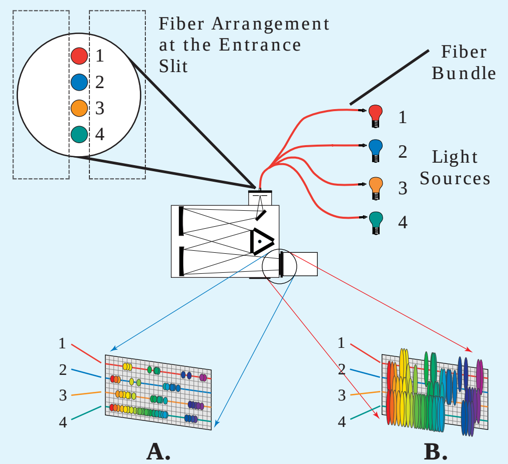


Figure 7: Collecting Multiple Spectra Simultaneously

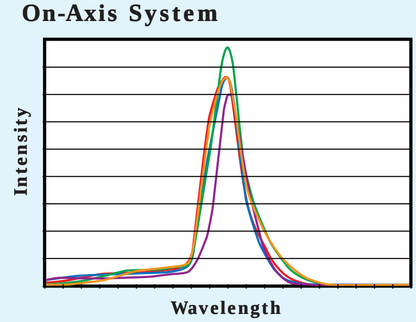


A four leg fiber bundle collects light from four different sources to the spectrograph and CCD detector.

A. With an imaging spectrograph the images at the focal plane/CCD are stigmatic, preserving both spatial and spectral information. This enables use of multiple inputs.

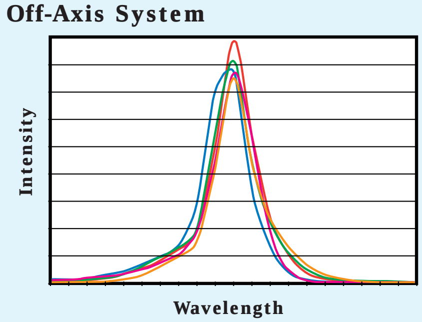
B. Conventional spectrographs have astigmatism, causing vertical line images at the focal plane/CCD. Multiple inputs overlap vertically and interfere with each other, severely limiting multiple input capabilities.

Figure 8: Spectral Resolution, On-Axis System



Spectral resolution varied from 0.13nm to 0.17nm fwhm across a 25mm wide focal plane for the on-axis instrument. This is a total variation of 0.04nm.

Figure 9: Spectral Resolution, Off-Axis System



Spectral resolution varied from 0.15m to 0.16m across a 25mm wide focal plane for the off-axis instrument, for a total variation of 0.01nm.

can be read out simultaneously without the signal from one fiber interfering with another if the vertical astigmatism is sufficiently reduced (See Figure 7). By employing toroidal optics in the spectrometer design, the vertical astigmatism in a 300mm focal length f/4 spectrograph can normally be reduced to ~120 microns or less on the optical axis. Spectrometers using this design are usually referred to as “imaging spectrographs.”

Extra vertical curvature of toroidal optics brings the tangential and sagittal focal planes together at the central axis (Refer to Figure 5). The focal planes are not parallel, however so they cross at this position forming an “x”. Placing an array detector on the tangential focal plane of an imaging spectrograph results in excellent spectral resolution with some astigmatism reappearing left and right of center. Conversely, placing the detector on the sagittal focal plane results in exceptional vertical image quality across the focal plane at the expense of spectral resolution for images left or right of center. In practice a detector could be placed on either focal plane, or in some compromise angle between the focal planes depending on the measurements being made, or if physical limitations exist.

Toroidal designs are also advantageous in the monochromator mode, in that with insignificant astigmatism on the central axis, no light is lost due to overfilling small solid state detectors such as those employing HgCdTe or InGaAs.

Spectral and Spatial Resolution as an Imaging Spectrograph:
We measured the spectral and spatial resolution at multiple points across the focal plane. For spectral resolution measurements, we illuminated a 25µm wide by 4mm high slit aperture with a mercury light source. The 435.8nm spectral line was selected for the tests and a Princeton Instruments CCD featuring a 1024 x 256 array of 26µm x 26µm pixels was used as the detection system. **The CCD was positioned on the tangential focal plane for best spectral resolution for both tests.** Spatial measurements were made by illuminating a line of seven 200µm diameter fibers with the mercury lamp. The size of the focal plane was approximately 26.6mm wide by 6.7mm high. For both tests. we positioned the image of 435.8nm emission from the lamp on the central axis and then 6 mm and 12mm to the left and right. While we were expecting to see some spatial degradation in both systems as we scanned the image away from the optical axis, we were looking to see if one design produced noticeably better results as the grating angle was changed. We translated the 435.8nm line from 12mm to the left of the central axis to 12mm to the right for these measurements.

Spectral Resolution:
Table 1 shows measured spectral resolution across the tangential focal plane. As can be seen from Figures 8 and 9, the observed differences in spectral resolution were within expected manufacturing tolerances for

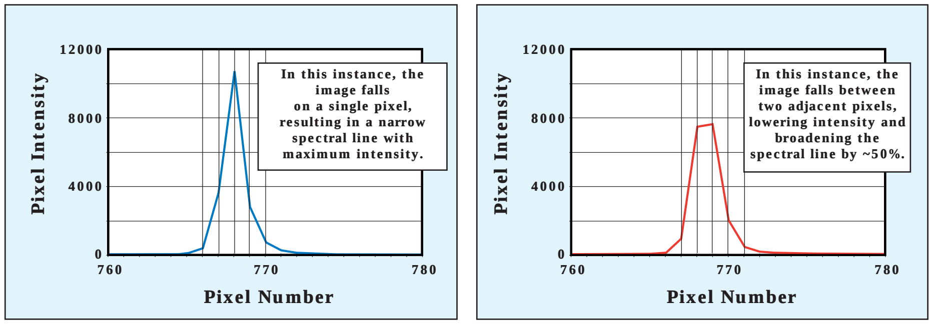
the systems. All spectral lines measured had fwhm values corresponding to ~2.5 to 3 pixels, which is within the expected pixel limited performance of CCD detection systems. It is interesting to note that while the on-axis spectrograph achieved the best measured spectral resolution (0.13nm at 12mm left of the focal plane center), this is also the position with the highest degree of astigmatism.

Further, the effects of image position on an individual pixel had a far more significant impact on spectral resolution measurements than any differences that might be attributable to the grating rotation technique. As Figure 10 shows, there can be as much as a 50% difference in apparent FWHM for the same spectral line centered on a pixel or positioned between two adjacent pixels.

Spatial Resolution:
In order to evaluate the vertical astigmatism, we measured the elongation of the image of the full line of fibers described above. The actual length of the illuminated area of the fiber bundle was 1.7mm. We subtracted that value from the measured image size in the focal plane. This measurement was made by counting the number of pixels covered by the image to the 1% peak intensity level. At this level there is virtually no cross-interference from one source input to another. The measurement was limited to the accuracy of using 26µm pixels as the measuring increment. The difference in the measured height of the image from the actual length of the bundle was attributed to the astigmatism and inherent wavelength dependent magnification through the system.

Ray Trace Analysis:
After performing our measurements, we then ray traced the optical systems to validate our results. Table 2 shows measured and calculated results. The ray tracings show that there should be a small overall advantage to the off-axis design in that the maximum overall astigmatism is smaller. While this calculation seems to be in agreement with the claim stated in the patent, we would not consider this theoretical advantage important in short focal length systems as the differences seem to be within manufacturing tolerances. It may be more apparent and significant in longer focal length systems, 500mm and larger.

Figure 10: Pixel Limited Spectral Resolution:



Effect of Image Position on a CCD to Apparent Spectral Resolution
The two scans above are spectral curves from the same well-focused image through a spectrograph onto a CCD. The blue line is a spectral curve from the image centered on a CCD pixel. The red line is a spectral line from the same image falling between two adjacent pixels. The difference is an apparent change in spectral resolution of ~50% and a drop in peak intensity. This is not a limitation of the spectrograph, rather a "pixel limited" situation.

Table 1: Spectral Resolution (nm) with 25µm Wide Entrance Slit

	12mm left	6mm left	Center	6mm right	12mm right
on-axis	0.13	0.15	0.16	0.14	0.17
off-axis	0.16	0.16	0.15	0.15	0.15

Table 2: Vertical Astigmatism In Millimeters

	12mm left	6mm left	Center	6mm right	12mm right
on-axis measured	0.96	0.44	0.12	0.34	0.74
off-axis measured	0.79	0.42	0.12	0.34	0.74
on-axis traced	0.78	0.41	0.09	0.31	0.73
off-axis traced	0.73	0.40	0.08	0.28	0.68

Conclusions:
For this evaluation, the off-axis design achieved superior spectral resolution as a scanning monochromator, with a flatter focal plane as a spectrograph. The practical differences between the two designs, however were small and within normal manufacturing tolerances. While there may be theoretical differences in ultimate performance for spectrometric measurements with off-axis vs on-axis grating rotations, considerations of normal aberrations in fast short focal length systems and pixelation on CCD detectors are far more significant in determining the limiting performance of these systems. We further believe that careful alignment and focusing of the total system has a more dramatic impact on performance than the grating rotation technique chosen.

With no significant performance differences between on-axis and off-axis techniques, one should look at other factors to decide which instrument is right for the application. These could include:

- **Track Record:** Is the instrument proven? How many are in operation?
- **Fundamental Quality:** What warranty is offered?
- **Operation:** How easy is the system to set up and operate?
- **Computer Control:** How easy is the instrument computer control?

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