Comparing modelling techniques when designing VPH gratings for BigBOSS

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ABSTRACT

BigBOSS is a Stage IV Dark Energy instrument based on the Baryon Acoustic Oscillations (BAO) and Red Shift Distortions (RSD) techniques using spectroscopic data of 20 million ELG and LRG galaxies at $0.5 \leq z \leq 1.6$ in addition to several hundred thousand QSOs at $0.5 \leq z \leq 3.5$. When designing BigBOSS instrumentation, it is imperative to maximize throughput whilst maintaining a resolving power of between R=1500 and 4000 over a wavelength range of 360-980 nm. Volume phase Holographic (VPH) gratings have been identified as a key technology which will enable the efficiency requirement to be met, however it is important to be able to accurately predict their performance. In this paper we quantitatively compare different modelling techniques in order to assess the parameter space over which they are more capable of accurately predicting measured performance. Finally we present baseline parameters for grating designs that are most suitable for the BigBOSS instrument.

Keywords: VPHG, spectroscopy, BigBOSS

1. VPH GRATINGS IN ASTRONOMICAL INSTRUMENTATION

The application of dichromated gelatin holographic transmission gratings to spectroscopy first proposed in 1995[1] and the application of this technology for astronomical instrumentation was proposed in 1998.[2] Since this time they have been used in a number of spectrographs in many different forms and environments, including: VPH grisms operated at cryogenic temperature in MOIRCS, a Cassegrain near-infrared instrument of the Subaru Telescope;[3] Apache Point Observatory Galactic Evolution Experiment (APOGEE) spectrograph which uses large, 304×508 mm, glass to accommodate an elliptically shaped clear aperture of 290×475 mm[4] ; FORS2 at the VLT which has a number of high-throughput VPH grisms;[5] and are also being considered for instruments on many large telescopes, including the Wide Field Optical Spectrograph (WFOS) for the Thirty Meter Telescope (TMT).[6]

When designing astronomical instruments, VPH gratings offer many advantages compared to surface relief gratings since they offer an easily customized grating design. This customization results in gratings with high diffraction energies. The diffracting gelatin can then be encased in glass in order to protect the substrate and the glass can be anti-reflection coated. This results in a grating which can be easily cleaned and handled. The drawbacks are that the response is more strongly peaked, and that they do not work well at very low resolutions. However, since BigBOSS is a three arm instrument with a moderate resolution, the advantages of VPH gratings far outweigh the drawbacks.

2. DIFFRACTION BY A VPH GRATING

In VPH gratings the diffraction is due to a periodic variation of the refractive index of a film with a constant thickness as is shown schematically in panel (a) of Figure 1 for two types of VPH gratings: gratings with fringes which are both perpendicular and slanted with respect to the grating surface.

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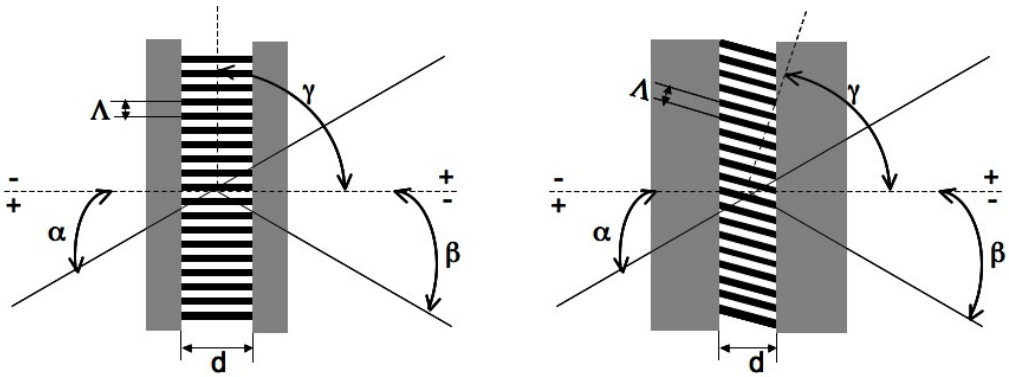


(a) (b)

Figure 1. Some possible VPH grating configurations showing Bragg condition diffraction, where where d is the thickness of the gelatin, ν is the grating frequency, α is the angle of incidence and β is the angle of diffraction. (a) Transmission grating with fringes perpendicular ($\gamma = 90$ degrees) to the grating surface (unslanted fringes). In this case the magnitude of α equals that of β for the Bragg condition. (b) Transmission grating with tilted fringes may reduce ghost images.[7]

As is shown in figure 1, the spacing of the fringe planes is defined as Λ or $1/\nu$ and this dictates the grating dispersion. The grating equation for a transmissive VPH grating is given by the standard grating equation:

$$m\nu\lambda = \sin(\alpha) + \sin(\beta), \tag{1}$$

where m is the order of diffraction, ν is the grating frequency, λ is the wavelength of light in free space, α is the angle of incidence in air, and β is the angle of diffraction in air (according to the sign convention for transmission, shown in both figures).

Light traversing a VPH grating is also affected by interaction with the fringes as it travels through the bulk or volume of the grating material. The depth of the grating volume, the intensity or contrast of the fringe structure, and the angular and spectral relationship of the incident light to the Bragg condition determine how much light goes into which order. These parameters are modified in order to optimize the efficiency of the grating.

The Bragg condition for a plane, parallel grating with fringes that are normal to the grating surface (the case shown in Figure 1) is given by:

$$m\nu\lambda = n2\sin(\alpha), \tag{2}$$

where ν is the frequency of the index modulation within the grating volume (where $\Delta = 1/\nu$), n is the average refractive index of the grating material, and α is the Bragg angle within the grating.

The Bragg condition for VPH gratings follows the same conditions as traditional gratings, so as the incident angle changes, the Bragg condition changes, and the peak efficiency moves in wavelength, this effect was utilized when designing gratings for the blue arm of the BigBOSS spectrograph and is discussed in section 5 .

2.1 Modelling VPH Gratings

Although the Bragg condition is the normal starting point when designing gratings, the diffraction efficiency also depends on the semi-amplitude of the refractive-index modulation Δn, and the grating thickness, d, in addition to the angle of incidence. Kogelnik[8] developed a two-wave, first order coupled wave analysis that can be used to estimate the first order efficiency of a VPH grating, using an approximation that is accurate (to within 1%) when

$$Q = \frac{2\pi\lambda d}{n\Lambda^2} > 10, \tag{3}$$

where λ is the wavelength d is the thickness of the gel, n is the index of the gel and Λ is the grating period.

When the grating design is outside of this limit, there are two main methods that are generally employed to theoretically model the diffraction efficiency: Rigorous Coupled Wave Analysis (RCWA)[9] and modal analysis.[10,11] Both of these methods involve complex computations, however, software exists to simplify the task. GSolver^{TM} is one such example which has been successfully used to predict the performance of VPH gratings. In this paper the performance of Kogelnik approximations and predictions made by GSolver^{TM} will be compared to Kasier proprietary software.

3. DESIGNING GRATINGS FOR BIGBOSS

Grating design is primarily driven by resolution requirements, however the angular dispersion also drives the requirement on the size of the grating. Gratings with a small angular dispersion result in a broad efficiency curve but are physically large, gratings with a large angular dispersion result in a more peaked efficiency curve but are physically small . Since resolution requirements are determined by science goals, this issue will be discussed first in section 3.1. The size of the gratings is discussed in section 3.2.

3.1 Resolution requirements

BigBOSS targets comprise of Emission Line Galaxies (ELG), Quasi-Stellar Objets (QSO), and Luminous Red Galaxies (LRG). Resolution requirements are driven by ELG observations since, at higher redshifts, it is necessary to resolve the [OII] and [OIII] doublet. The drivers of the resolution requirements are shown in table 1 and also how the current spectrograph design meets these requirements is shown in Figure 2.

Specification	Requirement	Wavelength	Reason	Object type
$\lambda/\Delta\lambda$(FWHM) - includes convolution of fibre size, optics, grating scatter CCD pixelation and detector effects	≥ 1500	360 – 555 nm	For redshifts less than z=.49, both [OII] and Hα are seen	QSO
	≥ 3000	555 – 656 nm	In this wavelength range the bright line cannot be Hα	ELG/LRG
	≥ 4000	656 – 980 nm	Must be able to resolve the [OII] doublet	ELG

Table 1. Resolution requirements for BigBOSS

The wavelength bands were adjusted in order to meet the maximum resolution at each wavelength without exceeding the requirements at other wavelengths within the bands in order to simplify the grating design and maximize the grating efficiency.

3.2 Angular dispersion requirements

Simple trigonometry can be used to estimate the size of the grating for a given angular dispersion, $\Delta\beta$, however a full Zemax representation of the spectrograph must be used to calculate this more accurately. As discussed above, for a given input angle and grating period, a larger $\Delta\beta$ will result in a smaller grating, however the efficiency curve will be more peaked than for a grating with a smaller $\Delta\beta$. This is due to the simple fact that as $\Delta\beta$ increases, the light at wavelengths that is further from λ_{Bragg}, is exiting the grating at angles that are further from θ_{Bragg} and consequently have a much lower efficiency. Therefore a balance must be made between cost and efficiency requirements.

An initial parameter space search using Kogelnik analysis allowed us to determine that gratings with angular dispersions less than 16.5° could be designed which met the minimum efficiency requirements. In order to predict the efficiency more accurately, these parameters were then used in simulations using GSolver^{TM} . Figure 3 shows

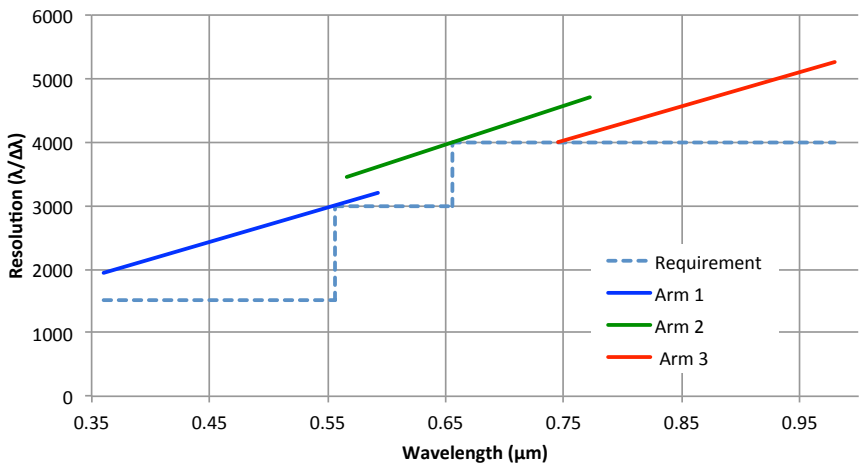


Figure 2. Wavelength bands have been selected so that each grating meets resolution requirements

the efficiency predictions as a function of wavelength for a range of gratings in this region. As is shown in this figure, gratings with the largest $\Delta\beta$ (16.5 degrees) have a peaked efficiency response, whereas gratings with the smallest $\Delta\beta$ (12.2) have a flatter efficiency curve across the wavelength band.

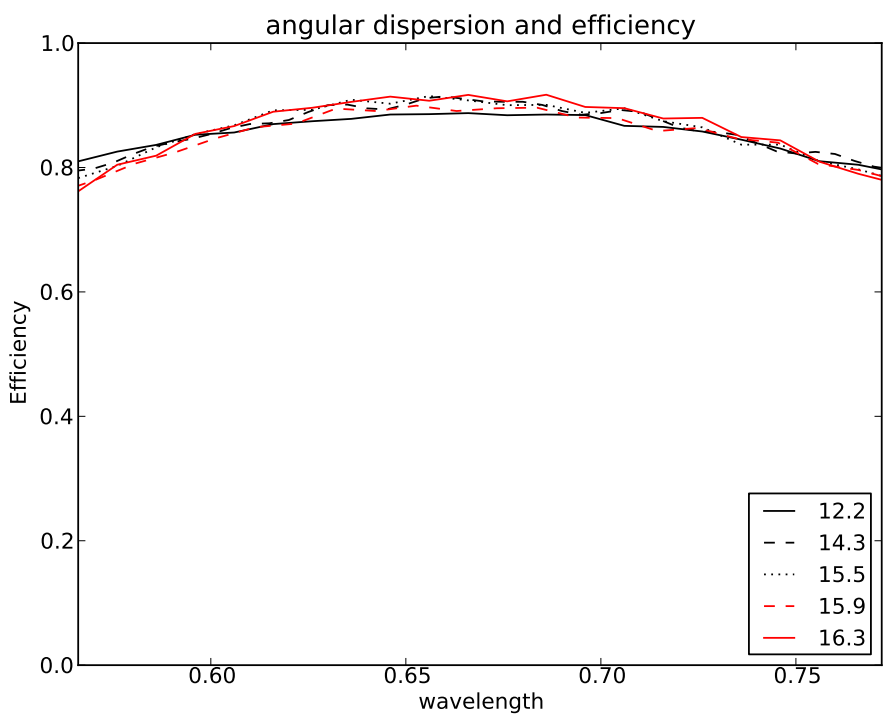


Figure 3. Grating design parameters were optimized for gratings with an angular dispersion less than 16.5°. This figure shows the results for an example grating for the red arm of the spectrograph with wavelength in units of microns.

4. MODELLING COMPARISONS

As stated in section 2.1, three methods were used in order to design and predict the efficiency of the gratings: Kogelnik analysis, GSolver^{TM} , and predictions made by James Arns. Kogelnik analysis was the first step in the design process since it is a simple model which can be used in order to predict where the peak in efficiency will occur and hence reduce the parameter space. GSolver^{TM} was then used to find the exact combination of gel thickness and index modulation which would produce the most efficient grating whilst remaining small enough to meet size requirements. Finally, predictions were made by James Arns at Kaiser using the same parameters in order to compare the different methods.

Figure 4 shows the grating efficiency as a function of wavelength. Since Kaiser normally guarantees that their gratings will be delivered to within 7-10% of their predicted values, the efficiency predictions of the other two methods were compared to these numbers. Figure 5 shows the percentage difference between the efficiencies predicted by Kogelnik analysis and GSolver^{TM} compared to Arns predictions.

GSolver^{TM} predicts the grating efficiency to within the manufacturing tolerances of Arns predictions over our entire wavelength band for our specific parameters. Kogelnik analysis predicts the correct shape of the curve and where the peak in efficiency occurs, however it does not predict absolute efficiencies well enough to be used in this project.

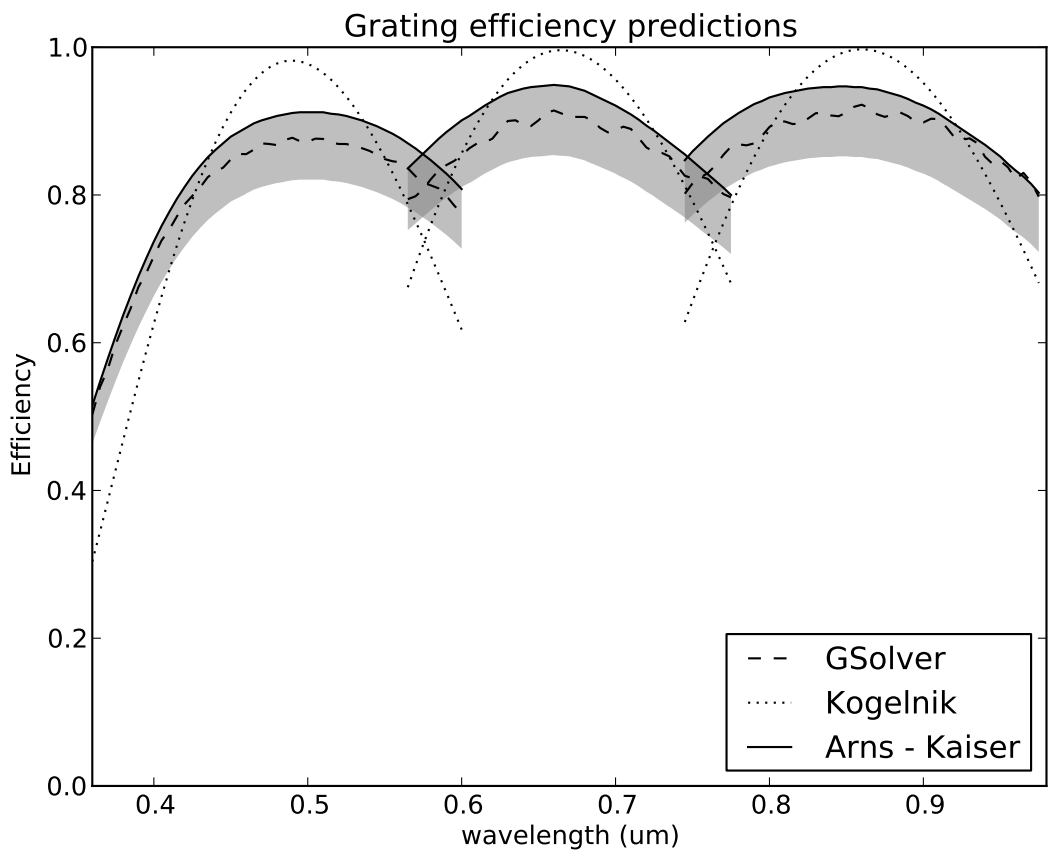
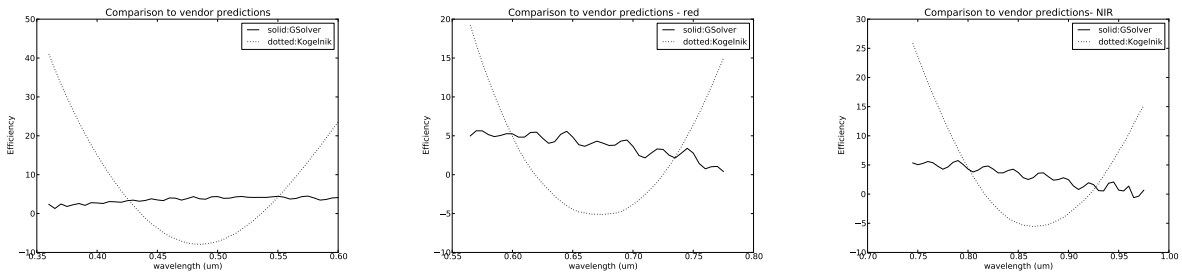


Figure 4. Comparison of modelling methods for one spectrograph design being proposed for BigBOSS. All gratings in this figure have an angular dispersion of $\Delta\beta$ =14.3 degrees



(a) (b) (c)

Figure 5. Percentage difference between calculations made by James Arns at Kaiser and those made using a Kogelnik analysis and GSolver^{TM} for the (a) blue arm, (b) red arm, and (c) NIR arm.

5. GRATINGS FOR THE BLUE ARM

Since the resolution requirements for BigBOSS are modest, it was relatively easy to design gratings for the red and near infra-red arms that met efficiency requirements. However, in order to meet resolution and size requirements it was not possible to achieve 80% efficiency across the entire blue band. In order to understand this problem, gratings were first designed which met efficiency requirements at the red end of the band, then, as is common when designing gratings in this wavelength region, the input angle to the grating was modified in order to tilt the efficiency curve and gain more throughput at the blue end of the band, at the expense of the efficiency at the red end of the band. This is shown as red lines in Figure 6 where the solid red line (A1) is the grating at the Bragg angle and the dashed red line (A2) is the same grating with light incident at a smaller angle. Rather than rotating the grating to equalize efficiency, it is also possible to design a grating with equal efficiency at both ends of the band but which does now meet the efficiency requirement of 80%. This is shown as a solid black line (B) in Figure 6. These curves were compared to the figure of merit of the spectrograph using BBspecsim and it was found that there was a small advantage to using grating B. This will be further investigated for the final spectrograph design.

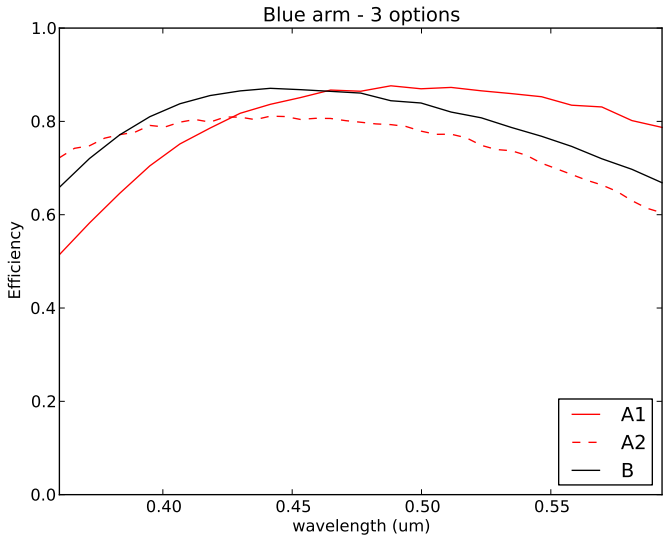


Figure 6. Grating options for the blue arm. Red lines show the same grating with different incident angles, the Bragg angle (A1) and the Bragg angle plus a few degrees (A2). Rotations around the Bragg angle allow gratings with unequal efficiency at the ends of the wavelength band to become more evenly distributed. The black line (B) shows the efficiency for a grating which was designed to have equal efficiency at both ends of the bands at the Bragg angle

6. CONCLUSIONS

It has long been known that VPH gratings can be successfully used in astronomical instrumentation and, indeed they have been used in many projects. As a result of this investigation, it has been shown that VPH gratings can be designed for BigBOSS which have a high throughput over the entire wavelength band. A comparison of modelling techniques has shown that GSolver^{TM} can be used to accurately predict the performance of the gratings within the manufacturing tolerances of Kaiser predictions. Predictions made using the Kogelnik analysis are not sufficient over line density and wavelength regime to accurately predict the performance, however it is a valuable tool to reduce the parameter space. More grating designs will be produced when the spectrograph design is finalised and slanted fringes will be added to the gratings in order to reduce the Littrow ghost and slightly reduce the size of the gratings.

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