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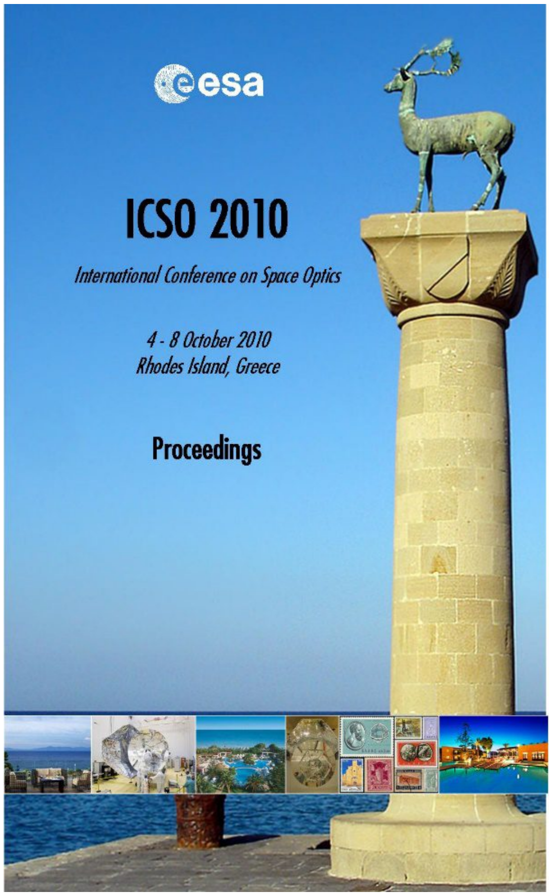

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APPLICATIONS OF IMMERSED DIFFRACTION GRATINGS IN EARTH OBSERVATION FROM SPACE.

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1. INTRODUCTION

A number of Earth-observation missions, particularly those aimed at monitoring atmosphere composition, require hyperspectral instruments measuring Earth reflectance and emission at very fine spectral resolution. Examples include instruments for ESA's Sentinel 5 mission, operating in the short-wave IR (SWIR) spectral region to quantify greenhouse gases, and also in the near-IR region (Oxygen-A band) to provide data on clouds, aerosols and atmosphere pressure. Conventional dispersive spectrometers, typically using diffraction gratings, are needed to provide data at moderate spatial resolution over large swath widths. Fine spectral resolution, together with the system aperture needed for radiometric resolution, tends to demand large beam diameters at gratings; this can lead to excessively large spectrometers, driven by the apertures of gratings and the associated collimators and camera lenses. This presents problems for accommodation of space-based spectrometers, particularly on small platforms.

Apertures, and complete spectrometer sizes, are reduced if the gratings provide high angular spectral dispersion (radians/nm) – this is a property of "immersed" gratings [1,2]. An immersed grating is a reflecting grating formed on a prism of refracting material, in which the incident and diffracted beams are both in the refracting medium. Instruments will typically use immersed gratings in silicon for short-wave IR bands, and silica for near-IR bands. This paper describes example designs for spectrometers using immersed gratings, and early results from a current development of immersed gratings are outlined.

2. THE NEED FOR FINE-RESOLUTION DIFFRACTION GRATINGS

2.1. Fine spectral resolution requirements in Earth observation – imaging spectrometers

Space-based instrument for Earth observation frequently use multi-spectral or hyperspectral information to quantify physical data products. In this paper, we are mainly concerned with instruments dedicated to monitoring atmosphere chemistry, using the absorption spectra of atmospheric gas species. Spectral signatures of gases have relatively fine structures (compared with those of solid or water surfaces), so that spectrometers with relative high resolving power are needed. Fourier transform spectrometers – providing very fine resolution – can be used in thermal IR bands, but grating spectrometers are usually found more appropriate for the spectral range from UV through visible, near IR (NIR: 700nm to 1000nm) and short-wave IR (SWIR: 1000nm to 2500nm). This spectral region is of particular use in measurement of atmosphere species in the troposphere, using absorption spectra in reflected sunlight.

In the UV/visible range, spectral resolution of around 0.5nm is useful, but in the NIR and SWIR bands, resolution of order 0.1nm is typically required. In the NIR band, the main region of interest is the Oxygen-A band, roughly from 750nm to 775nm, which is widely considered necessary for characterisation of aerosols and pressure. There is also current strong interest in use of the Oxygen absorption bands (Oxygen-B as well as Oxygen-A) to measure fluorescence of vegetation in sunlight – potentially a very useful indicator of photosynthetic activity – by detection of anomalous radiances in the deep absorption lines. In the SWIR region, several bands, each typically 50nm to 100nm wide, are used to monitor the greenhouse gases: CO_2, CO and CH_4.

The requirements for atmosphere monitoring typically include coarse spatial resolution – often in the range of several km – since gases are generally widely distributed. But frequent updates are desirable to measure changes over periods of days – or preferably hours. This means that instruments must cover wide swath widths – typically 1000 to 3000km from low-Earth orbit – so that a few hundred spatially-resolved areas can be covered on each orbit. A single instrument in low-Earth orbit (LEO), with a swath width approaching 3000km, can provide global coverage once per day; this is the approach proposed for the ESA Sentinel 5 mission. Eventually, much more frequent coverage will be considered desirable. A relatively expensive mission in Geostationary orbit – as proposed by ESA for the Sentinel 4 mission – would provide updates around once per hour, with the constraint that only about 1/3 of the Earth disc is observed. In the longer term, there is interest in a constellation of (preferably small) platforms in LEO. Measurement of vegetation fluorescence will probably aim for spatial resolution in the order 300m, and will also preferably cover swath widths over 100km – again requiring a few hundred spatial-resolution elements across the swath.

Imaging spectrometers – indicated schematically in Figure 1 – are normally used to provide the required combination of spectral and spatial coverage and resolution. A "telescope" forms an image of Earth on the entrance slit of a spectrometer, the light from the slit is collimated, dispersed by a grating, and re-imaged by a "camera" onto an area-array detector. The slit is imaged parallel to a detector row in each wavelength, and the spectrum of each spatially-resolved point is recorded by a column of elements. Silicon area arrays are used for UV, visible and NIR bands – mercury-cadmium-telluride (MCT) detectors currently offer the best performance for most SWIR bands.

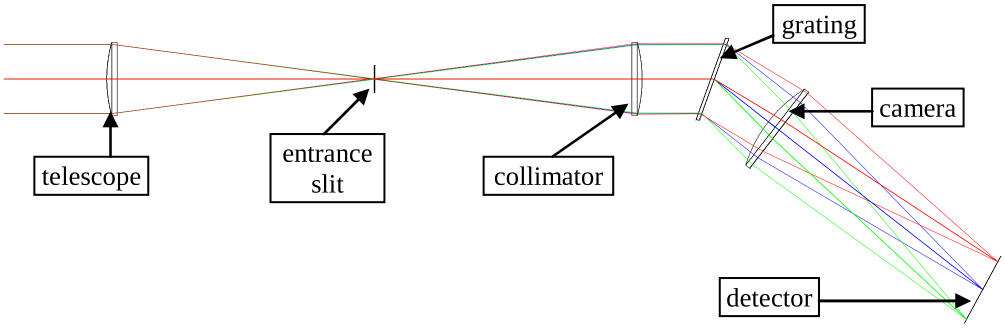

Figure 1 Spectrometer – schematic

2.2 The need for gratings offering high angular dispersion

The need for fine spectral resolution, together with requirements for high signal-to-noise ratios (SNRs) presents some basic problems for design of space-based imaging spectrometers. In particular, the gratings needed for fine resolution tend to be large, and they work with collimator and camera optics of equally large apertures. The relevant theory is briefly reviewed below:

The beam diameter at a grating can be calculated from the system étendue – the product of telescope aperture area and solid-angle subtense of the ground sample – which is needed to generate signal. Étendue (multiplied by the scene spectral radiance, spectral sample interval and optics transmission) defines the photon flux reaching the detector from each spatial/spectral resolution elements, and hence the system signal to noise ratio. Étendue is a useful concept in optical design, since it is the same at all well-defined system apertures through the system. Thus the necessary beam area at the grating is equal to the system étendue (required for signal to noise ratio) divided by the angular subtense (at the grating) of the spatial sample at the entrance slit. However the entrance slit width also constrains the spectral resolution of the spectrometer; the spectral resolution interval can be calculated by dividing the angular subtense of the slit by the angular dispersion of the grating (in units of radians per nanometre). Ignoring the relatively-marginal effects of non-circular apertures and anamorphic magnification, this implies that the beam diameter at the grating is inversely proportional to the grating dispersion:

grating_aperture = (entrance_aperture*SSA)/(dispersion*SSI)

where SSA is the spatial sample angle subtended at the entrance pupil of the system, SSI is the spectral sample interval, and grating dispersion is measured in radians/nm (and spectral resolution is in nm).

For an atmosphere chemistry mission, such as ESA's Sentinel 5, with a ground sample distance of around 7km (SSA is 0.009 radians for a platform at around 824km altitude), the entrance aperture diameter required to meet SNR requirements will be in the order of 2mm diameter, depending on optics transmission and detailed targets for spectral sampling etc. A typical diffraction grating, operating at angles of incidence and diffraction in the range 25° to 30°, in vacuum, will provide dispersion in the region 0.0014 radians/nm (0.08°/nm). This would imply a grating aperture diameter of about 120mm. This is of course quite feasible, but implies fairly large spectrometer optical systems for the NIR and SWIR bands. Instrument size is a consideration for all space programmes, but there will be increasing concern to minimise optics sizes for an approach using a constellation of atmosphere-chemistry instruments on small platforms in LEO. A similar calculation can be performed for an instrument measuring vegetation fluorescence on NIR absorption lines. In this case, high signal to noise ratios are required from relatively small ground-sample areas, so that the telescope entrance aperture needs to be in the order 100mm diameter. For 0.1nm spectral resolution, using conventional front-surface diffraction gratings, the grating aperture is in the region 300mm: this leads to prohibitively large spectrometers for Oxygen A and B bands.

Thus there are conflicting demands for fine spectral resolution (preferably 0.05nm or less) improved SNR and reduced instrument size. This provides the basic motive for investigation of gratings that provide intrinsically high angular dispersion. High dispersion must, however be combined with acceptable efficiency, since efficiency also affects the required étendue; low polarisation is also desirable.

2.3 Factors determining grating dispersion – the case for immersed gratings

Grating angular dispersion can be calculated using the formula:

$$\text{dispersion} = \mu(\sin(\theta) + \sin(\phi))/(\lambda.\cos(\phi)) \quad \text{radians/nm}$$

where μ is the refractive index of the dispersive medium, θ and ϕ are the angles of incidence and diffraction (on the same side of the normal), and λ is the wavelength of light in nanometres. This implies for example that the grating dimensions (and hence also the typical dimensions of the collimator and re-imaging lens) are inversely proportional to the refractive index of the dispersive medium. Over-simplifying somewhat, we can estimate that optics mass is inversely proportional to the cube power of the refractive index of the medium in which the grating operates. This is the basic case for immersion gratings, for which μ is significantly higher than 1. There are significant advantages in use of glass immersion prisms for NIR bands, and much larger advantages in use of silicon (with index 3.4) in SWIR bands.

Grating dispersion, and hence spectrometer size, are clearly also driven strongly by the angles of incidence and diffraction at the grating. For example, if typical angles can be increased from around 30° to around 60°, while retaining high efficiency, dispersion increases by a factor roughly 3 (and simplistically, instrument mass is reduced by a factor 3^3.) Ideally, we need to combine immersion with high efficiency at large angle..

2.4 Grating profiles – efficiency and stray light

In addition to high dispersion and efficiency, it is also generally very desirable to limit stray light generated by diffraction gratings; instrument data is used critically to analyse shapes of absorption lines, which can be affected by scatter of light in wavelengths at higher radiances. This tends to favour holographic methods for generation of grating profiles; in general the method involves recording a two-beam interference pattern in photo-resist, which generates very little random or systematic phase distortion. Following development, the photo-resist can be used directly as a grating, or simply replicated. However, several other processes are possible, including partial solution down to the substrate, and etching processes that may transfer the pattern into the substrate. In general, the grating requires a mirror coating to operate in reflection.

Photo-resist gratings (including replicas) generally have symmetrical shapes – typically approximations to sinusoidal, though generally modified by solution and etching processes. They can provide high efficiency in first-order diffraction when the grating period is similar to or less than the wavelength to be processed, when the incidence and diffraction angles are above 20° (on the same side of the normal). At these moderate or large angles, the grating is used in a single first order – apart from the zero order (mirror reflection) the other orders are evanescent so that selection of profile depth can generally concentrate a high proportion of power in the required order. Typically, this is achieved when the profile depth is in the region of quarter-wave, which gives low power in the zero order. As angles of incidence and diffraction are increased, to optimise angular dispersion, the grating period is reduced, so that high efficiency depends on profile depths that increase as a fraction of the period. This sets practical limits for dispersion of photo-resist-generated profiles (if we also demand high efficiency) since profile depths for photo-resists are limited to about 0.7 of the period: high efficiency is limited to incidence and diffraction angles up to around 30°.

In general, we much prefer efficiency at high angles. There is therefore interest in blazed gratings, which can provide high efficiency at large angles. For SWIR bands, this has lead to development of silicon immersed gratings, with blazed profiles produced by anisotropic etching – outlined in 3.1 below. For NIR bands, there is strong interest in lamella gratings (near square wave) with large profile depths produced by ion beam etching of silica; this is discussed in 3.2

3. IMMERSED GRATINGS FOR SWIR AND NIR SPECTRAL BANDS

3.1 Blazed gratings for SWIR by anisotropic etching of silicon

Blazed gratings have classically been produced by machining of substrates (or replication from machined substrates). The major disadvantage of mechanically-generated gratings is that they tend to produce stray light due to systematic pattern errors and surface roughness. However, this problem has been largely circumvented in current developments, particularly by SRON [3], using anisotropic etching. The process starts with a relatively conventional pattern generation in photo-resist, but the profile is finally generated by etching of silicon, using the crystal structure to generate sharply-defined facets defining a blaze at 55°. The gratings operate in high order, and require a metal coating, but the blaze provides efficiency over 50% in the selected order.

3.2 Deep profiles lamella gratings for NIR by ion-beam etching silica

Ion beam etching in fused silica has been used for some time to produce transmitting gratings, for example for the MegaJoule programme. However, if the gratings are produced on prisms of suitable shape, they can be used in internal reflection as immersed gratings [4]. There is extensive experience only in etching silica, which has a relatively low refractive index – 1.454 in NIR – and a low (though not insignificant) impact on dispersion. However, profile depths can exceed the period, so that high efficiency can be achieved at angles of incidence and diffraction of at least 50° to 60°. This gives a 200% advantage in dispersion, with respect to typical sinusoidal holographic gratings (if used at a high-efficiency limit on angles). The overall advantage in dispersion, and in potential reduction of spectrometer size, is dramatic.

SSTL, in collaboration with Horiba Jobin-Yvon, are currently performing a bread-boarding programme for ESA, which will develop and test a silica immersed grating. Parameters of the breadboard immersed grating are listed in Table 1.

Table 1 NIR immersed grating design parameters

Parameter	Value
Grating area	100mm x 100mm
Material	Fused quartz
Refractive index	1.454
Grating frequency	3226 c/mm (310nm period)
Grating profile shape	Lamella
Nominal profile depth	330nm
Nominal angle of incidence in SiO	61.12°
Nominal wavelength range	750nm to 775nm
Range of diffraction angles in SiO	53.08° to 57.55°
Angular dispersion in vacuum	0.26 °/nm (0.00454 radians/nm)

The grating will be generated on a flat plate of silica, and optically contacted to a silica prism, allowing light to reach the grating surface at the required angle in the refracting medium. The prisms is of course essential since the angles of incidence is above the critical angle for silica. The assembly works at close to the Littrow condition, with the diffracted beam leaving the prisms through the input face. Only the input/output face of the assembly is coated – a conventional anti-reflection coating. There are no transmitted diffraction orders (and only the first and zero orders in the medium), so that the grating face requires no mirror coating. The computed efficiency of the grating, in orthogonal polarisation planes, is shown in Figure 2.

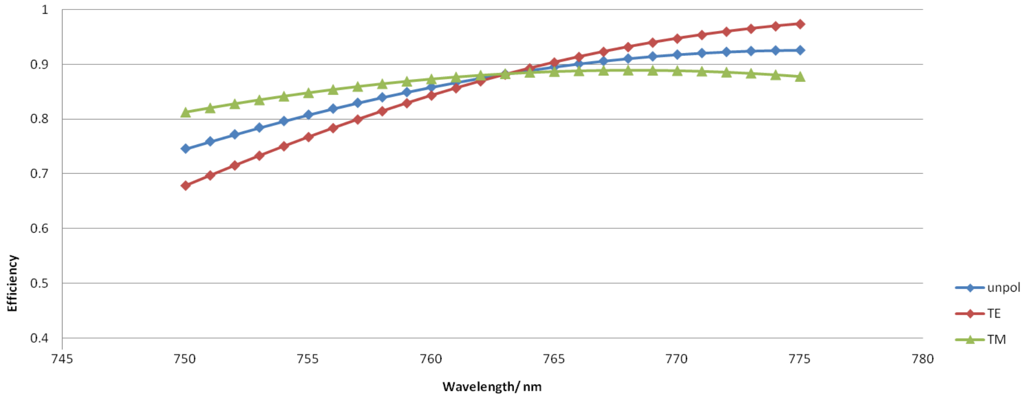

Figure 2 Computed efficiency of a silica immersed grating

4. EXAMPLE SPECTROMETER DESIGNS USING IMMERSED GRATINGS

4.1 NIR spectrometer design

An optical design for a spectrometer operating in the Oxygen-A band (750nm to 775nm) is shown in Figure 3. The telescope forms an image on the entrance slit; light from the entrance slit is collimated, and passes into the immersed grating via a small beam-shaping prism. After diffraction at the grating face, the beam is totally internally reflected at the input face of the immersing prisms. This provides a relatively efficient method by which the immersed grating can be operated close to the Littrow condition (with the input and diffracted beams on almost-reversed paths) without requiring that a common lens is used as both collimator and camera. The Littrow condition is generally preferred for efficiency; separate collimator and camera paths are preferred partly to separate the detector physically from the entrance slit, but mainly to avoid stray light that would be reflected by the collimator lens surfaces directly onto the detector.

This design has an aperture 100mm in diameter (telescope entrance pupil) truncated to 70mm in the section shown. The grating area is 100mm square, as in the development described in 3.2 above. It is a candidate for the FIMAS instrument (Fluorescence IMAging Spectrometer), which detects fluorescence from vegetation by anomalous radiances in the Oxygen absorption lines. It has a relatively fine spatial resolution, resolving 300m over a swath width of 150km from an altitude typically around 814km. A more typical spectrometer for the Oxygen-A band, used in atmosphere characterisation, would have a telescope with a much wider swath and a smaller aperture – however, very similar spectrometer configurations (slit to detector) could be used. The immersed grating allows a spectral resolution of 0.1nm over the 750nm to 775nm band.

The system is quite large, with a maximum dimension of 500mm rectangular aperture; mass of the optical head, including structure, will be in the region of 20kg. Although this is a fairly large optical system, note that the aperture of a conventional grating, providing the same étendue and spectral resolution, would typically be much larger – as indicated in 2.3 above. The immersed grating is necessary to provide spectrometer of acceptable size, when fine spectral resolution is demanded.

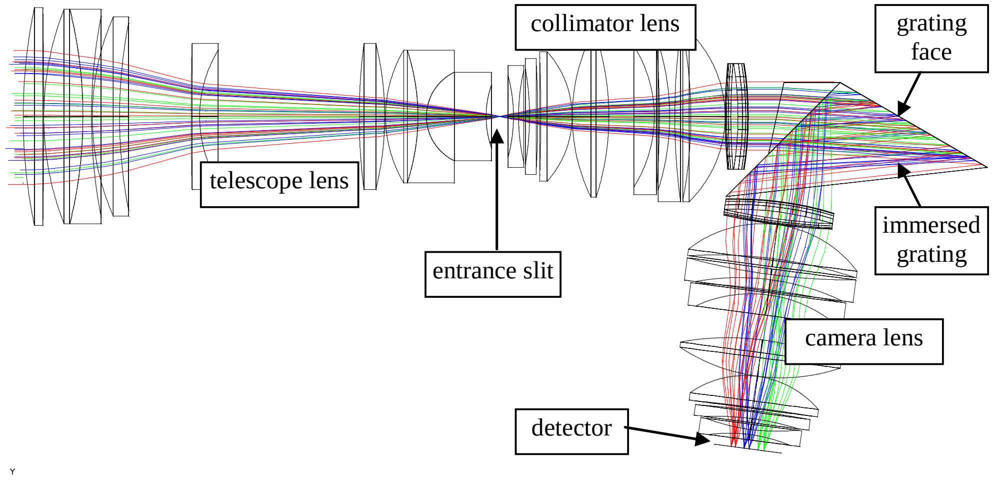

Figure 3 Optical design for an Oxygen-A band imaging spectrometer using an immersed silica grating

4.2 SWIR spectrometer design

A SWIR spectrometer design is indicated in Figure 4. The telescope, which is omitted from this diagram, forms a scene image on the entrance slit at long f/number – the beam from the entrance slit is therefore collimated by a lens system of long focal length, which is likely to be folded as shown. The collimated beam enters a silicon immersed diffraction grating. The beam passes through the input face at near-normal incidence and the angle of incidence on the grating face is nominally 60°. The design assumes the dimensions for the grating aperture 40mm x 30mm (the smaller dimension in the section shown). The grating frequency is nominally 480 c/mm. It covers the spectral band 2305nm to 2385nm in 5th-order diffraction. The grating is used quite close to Littrow condition, like the silica grating shown in Figure 3. However, the high refractive index of silicon magnifies the angular separation of the input and output beam in vacuum, so that it is unnecessary in this case to consider an efficient beam splitter to separate the input and output lenses. The camera lens, as before, images the dispersed slit image onto the detector.

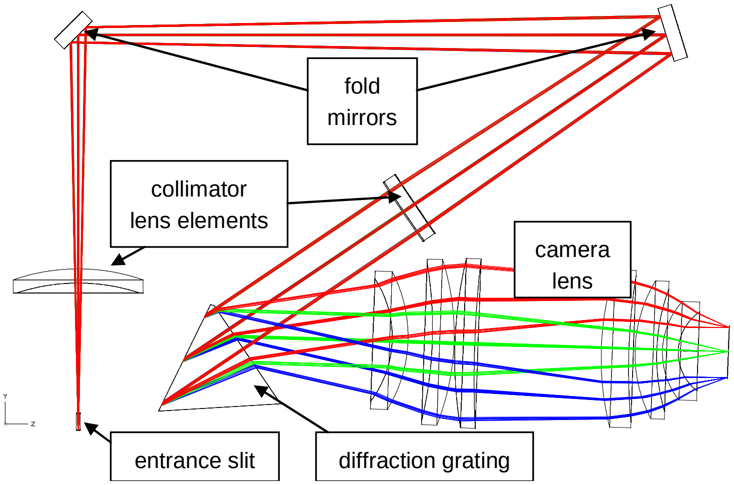

Figure 4 Optical design for a SWIR band imaging spectrometer using an immersed silicon grating

6. ACKNOWLEDGEMENTS

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