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VARIATIONS ON A THEME: NOVEL IMMERSED GRATING BASED SPECTROMETER DESIGNS FOR SPACE

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I. INTRODUCTION

We present novel immersed grating (IG) based spectrometer designs that can be used in space instrumentation. They are based on the design approach that aims to optimize the optical design using the expanded parameter space that the IG technology offers. In principle the wavefront error (WFE) of any optical system the most conveniently can be corrected in the pupil, where in the case of the IG based spectrometer, the IG itself is positioned. By modifying existing three-mirror based optical systems, which can form the main part of double pass spectrometer designs, a large portion of the WFE of the optical system can be transferred to the pupil and to the IG. In these cases the IG can compensate simple low order aberrations of the system and consequently the main benefit is that the mirrors that tend to be off-axis conical sections can be substituted by spherical mirrors. The WFE budget of such designs has only a minor contribution from the very high quality spherical mirrors and the majority of the WFE can be then allocated to the most complex part of the system, the IG. The latter can be designed so that the errors are compensated by a special grating pattern that in turn can be manufactured using the expertise and experience of the semiconductor industry.

II. IMMERSED GRATINGS

A. Immersed grating and its WFE budget

In the proposed designs we build on the expertise gained in our immersed grating development project, where together with our partners SRON, TNO and Philips we develop and manufacture an immersed grating in silicon for the Mid-infrared E-ELT Imager and Spectrograph, METIS ([1], [2]). Si is ideally suited as immersion material and these gratings can be used in space spectrometers that operate in the 1.2 µm - 6 µm wavelength range. Spectrometers are used for a wide variety of tasks in Earth observation from space, where fine spectral resolution is needed. Science observations, which necessitate very high spectral resolution tend to demand diffraction gratings immersed in different mediums (e.g. Si or Ge). Our proposed silicon immersed grating based spectrometers can be good candidates for e.g. monitoring greenhouse gases in short-wave IR bands 1600nm to 2400nm at better than 0.25nm resolution. Apart from NIR applications, they perform very well at the mid-infrared wavelength range as well.

Besides good transmission, single crystal Si also has beneficial anisotropic etching characteristics that allows for tailoring the groove profile to the specific grating requirements. The IG that is being developed at the moment for METIS is obtained via etching into the Si with the surface cut along the <100> crystal plane. The grooves thus will have a natural blaze angle close to 54.7 degrees depending on the anisotropic etch ratio. The angle of incidence on the grating will be close to this blaze angle. The grating is positioned at the bottom side of a Si prism (Figure 1). The grating is produced on a regular Si wafer that is bonded to the bottom surface of a Si prism. The light enters and exits the prism through the same facet. In our proposed spectrometer designs we use an IG with the characteristics described above. By doing that, we can be sure that we know the capabilities of the key component of the proposed designs.

In Figure 1 (right) the errors that contribute to the WFE budget of the IG are shown. #1 and #2 are the surface figuring of the front and back surfaces of the prism (before bonding and fusion of the prism with the wafer containing the grating), #3 is the total thickness variation of the wafer and finally #4 are the errors originate in the grating itself. The latter can be broken down into further four subgroups: line width variation after reactive ion etching, lithography distortion errors, lithography stitching errors and mask writing errors. Material inhomogeneity is not indicated, because for Si the material standard and properties as so extremely good that this error considered negligible.

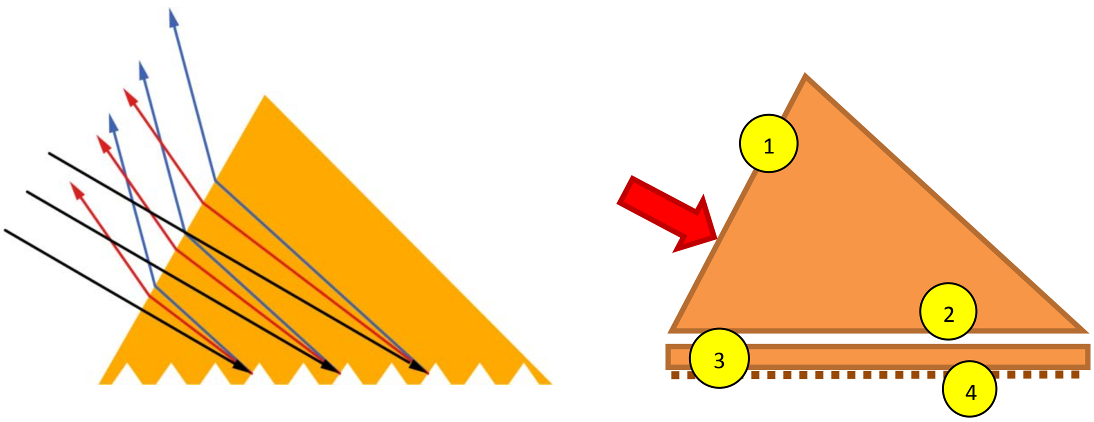

Figure 1 On the left the immersed grating principle is shown: light enters the prism through a polished entrance facet; after diffraction at the grating facet the dispersed light leaves the prism through the same facet. On the right the WFE contributors of the immersed grating are listed. The entrance surface is indicated with the arrow. #1 is the WFE of the front surface of the prism. #2 is the WFE of the back surface of the prism (before fusion of the prism with the wafer containing the grating). #3 is the WFE that results from the wafer total thickness variation (TTV, before fusion with the prism) and #4 is the WFE of the grating in reflection as measured from the air side of the grating. Material inhomogeneity is considered negligible.

III. NOVEL IMMERSED GRATING BASED SPECTROMETERS

A. General considerations and the novelty of the designs

Our intention is to design IG based spectrometers that can provide improvements with respect to existing spectrometers. The main benefit of these systems is that the spectroscopic resolution can be higher than in conventional echelle spectrometers. We investigate all-reflective optical designs and so the other advantage comes from the achromatic performance of such systems. The proposed spectrometers can be optimized to be used in a wide wavelength range, which is only limited by the transmission properties of the only refractive component, silicon.

We decided to focus on two and three mirror based double-pass systems. After the slit light is collimated and in the pupil, or in the vicinity of the pupil the immersed grating is positioned. After the diffraction that takes place in silicon, light is reflected back in a ‘close to Littrow’ configuration and focused on the detector by the same mirrors that were used for collimation. The double-pass systems have the advantage of compactness and due to the ‘close to Littrow’ arrangement high diffraction efficiency. In several designs performance can be improved by separating one of the double-pass mirrors (the one that is closest to the slit/detector) into two independent mirrors. In other designs the collimator or the camera optical path can contain one additional mirror. These systems become useful for focal-ratio conversion, when light that propagates from the slit and light that is focused on the detector should have different F-ratios. If only the same double-pass mirrors are used, these F-ratios will be very close and it is only possible e.g. to change the anamorphic ratio (different tangential and sagittal focal length) of the system by different mirror arrangement or deviation from the Littrow condition.

Different system geometries were investigated in order to decrease the spatial and spectral smile. As an example, two different three mirror anastigmat (TMA) configurations are shown in Figure 2. The TMA on the left has the slit and the detector next to each other, positioned along a plane perpendicular to the plane of the TMA mirrors. The TMA on the right has the slit and detector in the plane of the TMA mirrors. The latter configuration is advantegous because the ‘natural’ distortion of the TMA can be used to compensate for the curved slit images on the detector, which is a consequance of the geometry of the rays arriving from the grating. The detector image with the slit geometry is shown in Figure 3 for the two cases. The other advantage of the ‘in-plane slit and detector’ design is that the detector is not perpendicular, but tilted with respect to the chief ray, which means that the ghost from the detector can be driven away from the incoming optical path. The disadvantage is that the dispersion direction is also in the plane of the mask and detector and so oversizing of the mirrors is needed in that direction, which can make packaging and scattered light control more difficult.

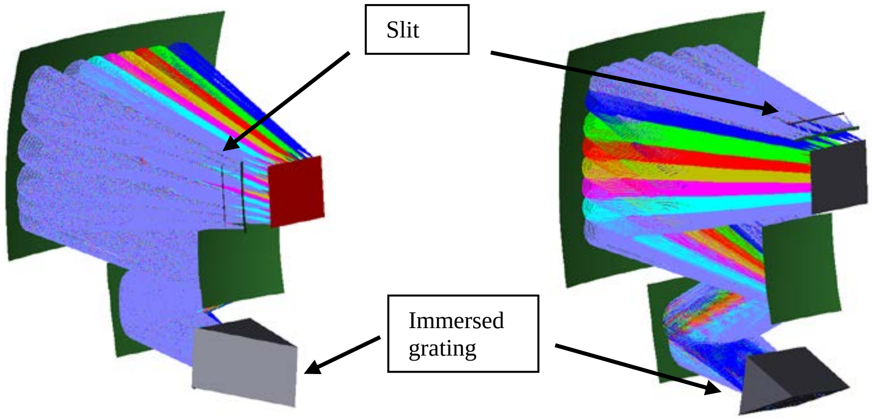

Figure 2 Layout of two IG based designs. On the left the slit and the detector are next to each other on the right they are in the plane of the TMA mirrors.

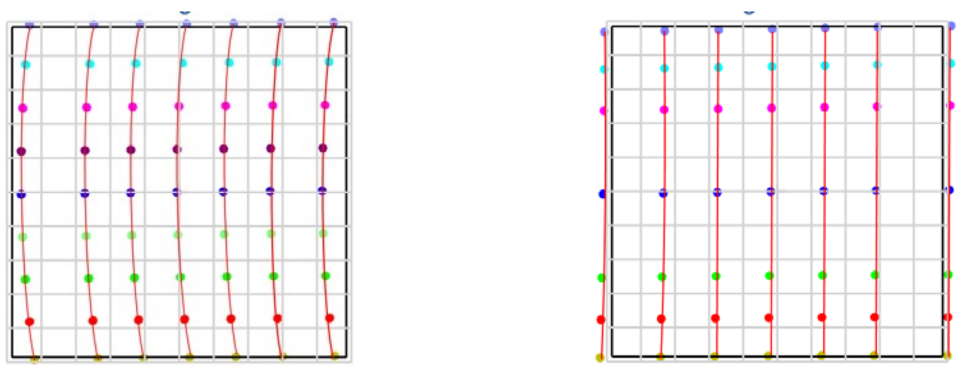

Figure 3 The slit geometry is shown for the two designs presented in Figure 2. By arranging the detector and the slit in the plane of the three mirrors of the TMA, straight slit geometry can be achieved.

The novelty of the proposed designs comes from two factors. One is the optimization technique. We investigated several TMA and Schwarzchild based two-mirror designs and re-optimized them in order to achieve the best possible RMS WFE on the detector. We created an optimization method whereby the optical system has the maximum degrees of freedom (DOF) possible. During optimization, the difficulty usually comes from the need to achieve an un-obscured system, while maximizing optical performance. One solution is to carefully select the off-axis angle of the field-of-view (FOV) and eccentricity of the pupil with respect to the axis of symmetry of the system. We improved the optical design by creating a 'floating' model, so that these two parameters are actually variables and the mirrors have the possibility to 'float' around during optimization. Naturally, constraints had to be set in order to avoid obscuration by the mirrors, but knowing the pupil size, the plate scale on the detector and the approximate footprints on the mirrors, the limiting conditions can be set in a way that the system stays un-obscured.

Other factor that provides novelty is the optimized grating pattern that makes possible to design optical systems that are easier to manufacture and more feasible to build. Basically, in these designs we shift complexity from the mirrors to the immersed grating pattern. During the optimization process we use the experience that we gained in our previous projects, where we were focusing on freeform mirror optimization methods ([3], [4]). Our optical design process is as follows. In a first optimization step we design an all-reflective IG based spectrometer that have very good optical performance, but the mirrors are still off-axis conics/aspheres. These are very difficult and costly to make, particularly in regard to surface figuring requirements (15-25nm RMS). In the second optimization run we convert as many mirrors from off-axis conics/aspheres into spherical mirrors as possible, while compensating the WFE of the system in the pupil. We achieve the latter by optimizing the grating pattern so that it can compensate low order aberrations. By e.g. using a linear line width variation, astigmatism can be compensated (in one direction) in the system. More complex grating patterns can compensate any kind of low order aberrations. We create spherical mirror based systems in order to improve the manufacturability of the optical components. There is no need for complex and very expensive manufacturing processes e.g. diamond turned aluminium mirrors with nickel plating and post polishing. Additionally, on the spherical surfaces lower surface figuring errors can be achieved leading to a better balanced WFE budget.

Based on the application, different requirements can be drawn and the system should satisfy those requirements. In the following we present the design evolution for one specific optical system, but the modifications of the proposed system is possible. Slit length, pupil size, F-ratio can be changed and the system can be re-optimized if necessary.

B. First optimization – system with off-axis conics

In the following we present a double pass TMA based spectrometer design that contains the immersed grating presented in Section II. The design is optimized for 4.65 µm wavelength (4.626 µm - 4.681 µm falls on the detector) and provides a spectral resolution of 50 000 (we don't consider here sampling of detector pixels). It has a telecentric slit with a length of 36mm and numerical aperture of 0.0625 (which corresponds to F8). The size of the pupil is 30mm and the F-ratio on the detector is F7.5. It is an all-reflective optical design and the TMA mirrors are off-axis conic sections. The grating surface of the IG has a size of 40mm x 70mm, so it fits on an industry standard 100mm diameter Si wafer. The grating lines are parallel with the short side of the rectangular grating surface. The layout and the RMS WFE in waves are depicted in Figure 4. It has a diffraction limited performance for the modelled wavelength range. Since it is an all-reflective design, it stays diffraction limited down to 2.3 µm, where it can still provide a spectroscopic resolution of R~50 000. Below 2.3 µm the spectroscopic resolution starts to degrade, but still at 1.6 µm wavelength it is around R~35 000.

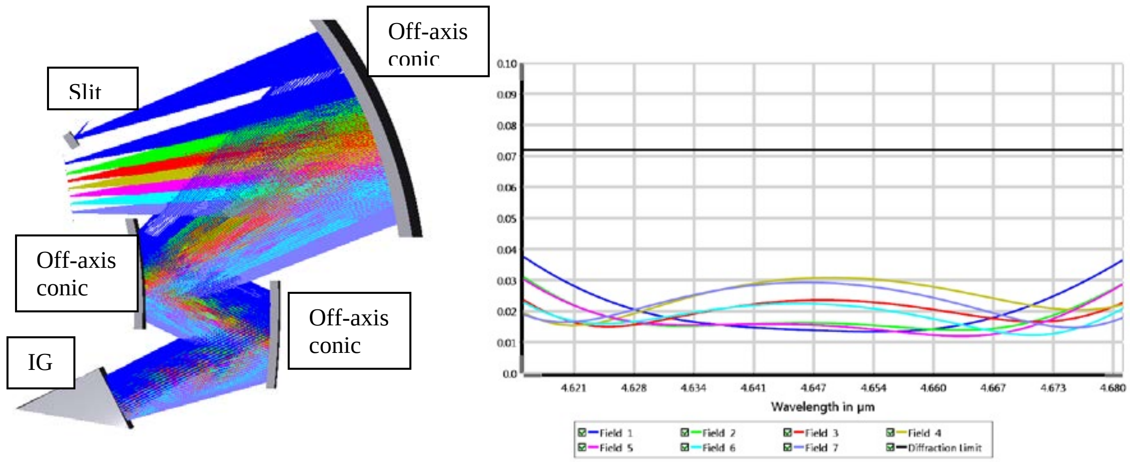

Figure 4 Layout (left) and RMS WFE in waves (right) of the proposed IG based spectrometer after the first optimization step. Diffraction limit is indicated by a horizontal line.

C. Second optimization – system with two spheres, one conic

The optical system is re-optimized, using the 'floating TMA' method described previously. Going from the IG based design consisting three conics, the primary mirror (the largest one) and the tertiary mirror (closest to the IG) are transformed into spherical mirrors at the expense of some of the WFE. In this design the secondary mirror of the TMA is still a conic section. The result is shown in the Figure 5. Especially for the longer wavelength range, the WFE increased and as a result this optical design has a degraded performance compared to the previous one. Essentially, the good image quality of the previous design was traded for better manufacturability of two mirrors.

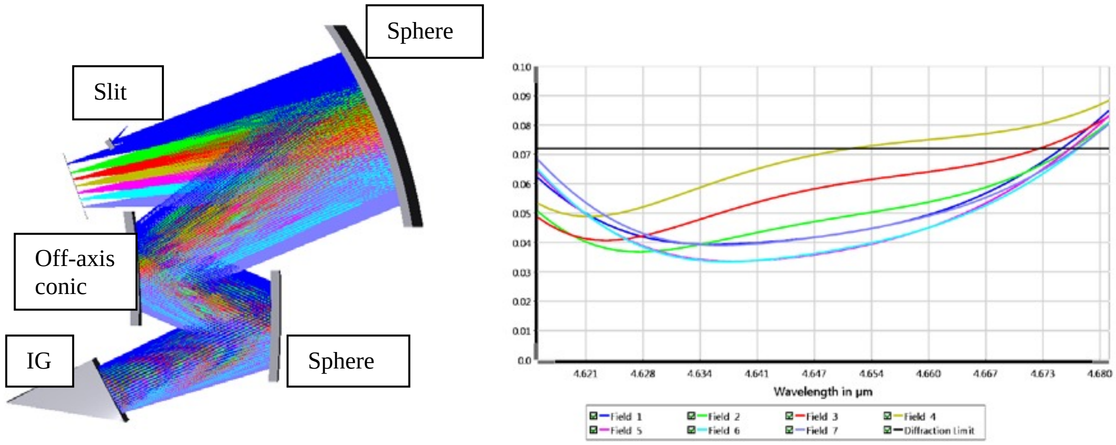

Figure 5 Layout (left) and RMS WFE in waves (right) of the proposed IG based spectrometer after the second optimization step. Diffraction limit is indicated by a horizontal line.

D. Third optimization – system with two spheres, one conic and an optimized grating pattern

Finally, in the last re-optimization step we optimize the grating pattern itself, so that it compensates for some of the low order WFE in the optical system. The system layout and the RMS WFE are shown in Figure 6. Looking at the RMS WFE it becomes apparent that the RMS WFE provided by the original three conics based TMA can be recovered with this system. The surface deformation, seen from the Littrow direction is shown in Figure 7. It is decomposed into Noll type Zernike polynomials between z5 and z11 (astigmatism, coma, trefoil and spherical aberration); the results are depicted in Figure 8. The most dominant aberration that is compensated by the IG is astigmatism. The design has a diffraction limited performance for the modelled wavelength range and similarly to the three-conics based design, it stays diffraction limited down to 2.3 µm, where it has still a spectroscopic resolution of R~50 000. Below 2.3 µm the spectroscopic resolution starts to degrade, at 1.6 µm wavelength it is around R~35 000.

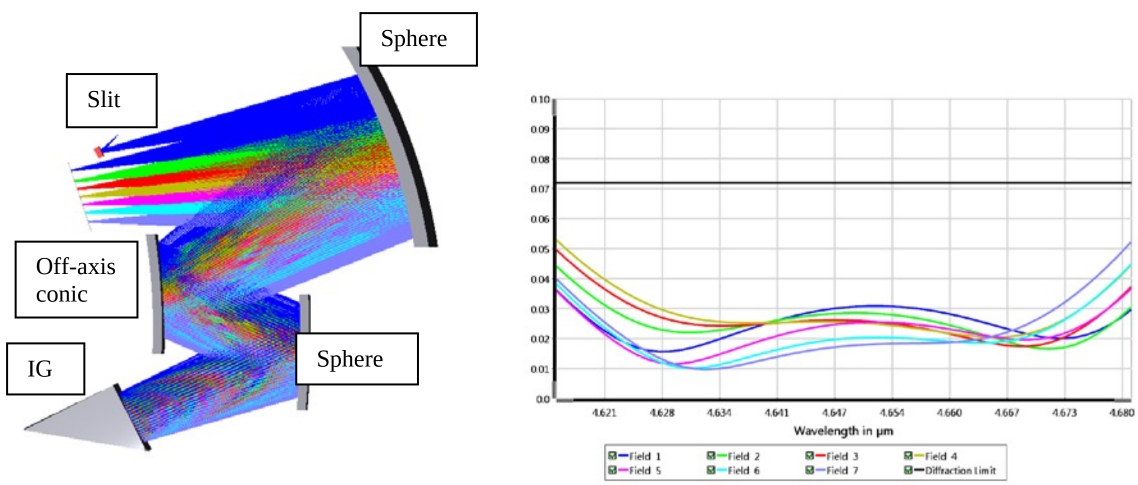

Figure 6 Layout (left) and RMS WFE in waves (right) of the proposed IG based spectrometer after the last optimization step. Diffraction limit is indicated by a horizontal line.

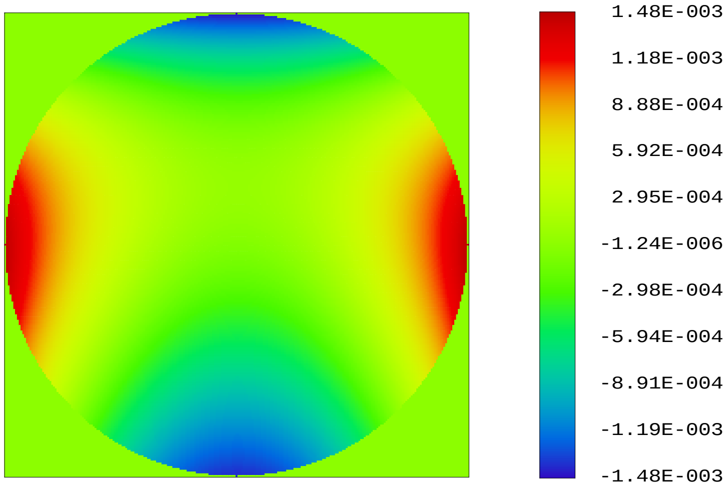

Figure 7 The surface deformation of the grating looking from Littrow direction is shown. It is the result of a variable (x,y) grating pattern that creates these low order aberrations. The units are in mm. The PV surface deformation is less than 3 µm.

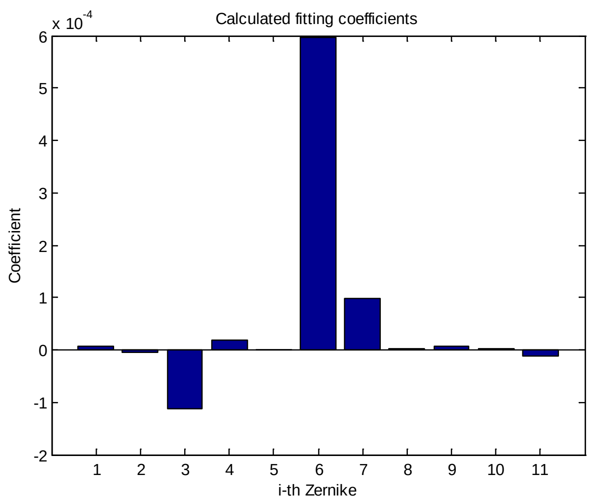

Figure 8 The Zernike decomposition of the surface deformation (Figure 7) is shown. The coefficients show the RMS surface deformation of each Zernike term in mm. The most dominant aberration is astigmatism (RMS 0.6 µm surface deformation).

V. CONCLUSIONS

We presented innovative, immersed grating based optical designs for space based spectrometers. Using novel optimization techniques we optimized double-pass two- and three-mirror designs for best optical performance (WFE vs. wavelength). We presented a TMA design that has diffraction limited performance above 2.3 µm and capable to achieve a spectral resolution of R~50 000. Below 2.3 µm the spectroscopic resolution starts to degrade, but still at 1.6 µm wavelength it is around R~35 000. We converted two of the three off-axis conic mirrors to spherical mirrors in order to significantly improve the manufacturability of the system, while the WFE we compensated by an optimized grating pattern on the IG. The WFE budget of the design has only a minor contribution from the very high quality spherical mirrors and the majority of the WFE can be allocated to the most complex part of the system, the IG. The optimized grating pattern can be manufactured using the expertise and experience of the semiconductor industry.

The optical systems and processes presented here will have to be developed further with more thorough analyses in order to satisfy the demanding requirements. Currently, we investigate how to improve the spectral and spatial smile in these systems. Also we intend to study the effect of the designed grating patterns on diffraction efficiency and ghosts. Finally, our aim is to design test and verification setups and configurations for these IG based spectrometers.

~~VI.~~ ACKNOWLEDGEMENTS

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