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CARBONSAT INSTRUMENT PRE- DEVELOPMENTS: TOWARDS MONITORING CARBON DIOXIDE AND METHANE CONCENTRATIONS FROM SPACE

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CarbonSat was a candidate satellite mission in the frame of ESA's Living Planet Programme, which targeted high-precision measurements of carbon dioxide (CO_2) and methane (CH_4) concentrations from space. Although not selected for implementation as ESA's eighth Earth Explorer, the instrument concepts developed during the Phase A/B1 studies may serve as a starting point for the development of a space component as part of a future observing system for monitoring greenhouse gases. The CarbonSat concept distinguishes itself from previous space missions, like JAXA's Greenhouse Gas Observing Satellite (GOSAT) and NASA's Orbiting Carbon Observatory (OCO-2), by combining a wide swath (250 km) with high spatial sampling of (6 km^2). This combination allows for separately addressing both, biogenic and anthropogenic fluxes of CO_2 and CH_4 at regional to local scales. The challenging mission objectives and the need to quantify small local differences in concentrations of greenhouse gases lead to demanding radiometric and spectral requirements for the instrument. Detailed instrument concepts were developed by two independent industrial consortia, resulting in consolidated designs for space-borne push-broom imaging grating spectrometers. Despite the similarity of the detection concepts, different choices were made in terms of key technologies, such as diffraction gratings and Sun diffusers. In order to address the specific need of high single-measurement accuracy at high spatial resolution over non-uniform scenes, both consortia devised hardware solutions based on so-called slit homogenisers. The above components have been subject to comprehensive breadboard studies, in order to mitigate development risk and raise the Technology Readiness Level (TRL). This paper provides an overview of these pre-development activities, with emphasis on the selected technologies for diffraction gratings. Laboratory test results for key performance parameters, such as efficiency, polarisation sensitivity and straylight, are shown. In addition, the baseline technologies for solar calibration (Sun diffuser) and non-uniform scene mitigation (slit homogenisers), as well as the corresponding breadboards of these components will be presented.

I. INTRODUCTION

The European Space Agency's Earth Explorers (EE), as part of its Living Planet Programme, are research missions designed to address key scientific challenges while demonstrating breakthrough technology in observing techniques. In 2012, ESA selected two missions as candidates for launch as the eighth Earth-Explorer mission (EE-8): The FLuorescence EXplorer (FLEX), targeting space-borne measurements of vegetation fluorescence, and the Carbon Monitoring Satellite (CarbonSat), dedicated to global measurements of greenhouse gas concentrations. These two missions were subject to feasibility studies carried out by two independent industrial consortia. These phase A/B1 studies included a comprehensive pre-development programme and dedicated breadboard activities for critical components. At the User Consultation Meeting in Krakow in 2015 [1] the FLEX mission was recommended for implementation as EE-8, which was endorsed by the Programme Board for Earth Observation in December 2015.

Although not selected as Earth Explorer, the CarbonSat concept is still regarded as a starting point for the development of a space-borne component as part of a global observing system for greenhouse gases. The European Commission has assembled a task force of experts to develop concepts for a global observing system targeting fossil CO_2 emissions [2]. This observing system will be comprised of multiple components, including a network of ground-based remote sensing (TCCON) [3] and in-situ stations, as well as atmospheric chemistry and transport models. The scope of the system calls for a space component providing continuous measurements of CO_2 concentrations with global coverage.

While anthropogenic emissions shall be the focus of the future observing system under study, previous and current space-borne instruments are designed to target biogenic fluxes of greenhouse gases. Measurements of CO_2 and CH_4 concentrations from space were pioneered by SCIAMACHY on board of Envisat in 2002 [4]. After the launch failure of NASA's Orbiting Carbon Observatory (OCO, [5]) in 2009, JAXA's GOSAT became the first dedicated mission to target CO_2 and CH_4 measurements from space [6], followed by OCO-2 in 2014 space [7]. These missions significantly increased the accuracy (~0.5 ppm), precision (~1 ppm) and spatial resolution (~ 3 km^2) of CO_2 measurements. However, due to the relatively small swath (OCO-2) and sparse sampling (GOSAT) they are not suited for quantifying emissions from point sources, such as power plants or large cities.

In contrast, the CarbonSat concept, which was described in [8], is based on continuous imaging of CO_2 concentrations, combining a wide swath (~240 km) with high spatial sampling (6 km^2) at high accuracy and precision. The key system requirements of the CarbonSat mission are listed in Table 1.

During the phase A/B1 studies the ability to detect plumes of CO_2 and CH_4 from point sources was demonstrated, making the concept particularly promising for observing anthropogenic emissions. The technologies developed during the EE-8 pre-development activities are therefore regarded as highly relevant for a future space-borne CO_2 mission, possibly in the frame of the Copernicus programme.
This paper presents selected results of the breadboard studies for CarbonSat, carried out by the two industrial consortia led by Airbus Defense and Space (ADS) and OHB. First, the two instrument designs are presented in Section II, followed by a brief description of the detector technology for the Short-Wave Infrared (SWIR) bands, which was commonly selected for both designs. Subsequently, the different solutions for diffraction gratings are compared and results of the characterization campaigns in terms of efficiency, polarization sensitivity and straylight are presented. Finally, we describe the so-called slit homogenizer assemblies, which have been developed to mitigate the impact of scene non-uniformity (clouds and albedo contrast) on radiometric accuracy. The paper concludes with an outlook on further developments, which are deemed to be relevant in the context of a future space-borne CO_2 monitoring instrument.

Table 1: Key system requirements of the CarbonSat mission.

SNR @ Lref (dark reference radiance)	NIR: 150; SWIR-1: 160; SWIR-2: 130
Spectral resolution (3 times sampled)	NIR: 0.1 nm; SW1: 0.3 nm; SW2: 0.55 nm
Swath width (coverage)	Minimum 180 km; Breakthrough 240 km; Goal 500 km
Spatial sampling distance (SSD)	2 km (ALT) x 3 km (ACT)
Spatial co-registration	15% of ACT SSD (NIR-SWIR)
Integrated Energy	>70% within spatial sample
Absolute radiometric accuracy	NIR: 2%; SWIR: 3%
Relative radiometric accuracy	0.5% (spatial and spectral)

II. MISSION CONCEPT AND INSTRUMENT DESIGNS

The CarbonSat mission concept is based on a push-broom imaging spectrometer on board of an agile satellite platform in a sun-synchronous orbit. The instrument performs spatially co-located measurements of Earth reflectance in three different spectral bands, at high to medium spectral resolution: Near Infrared (NIR, 747-773 nm @ 0.1 nm), SWIR-1 (1590-1675 nm @ 0.3 nm) and SWIR-2 (1925-2095 nm @ 0.55 nm). The agility of the platform is required to point the instrument field-of view towards the area of specular reflection over water in the so-called sun-glint mode, which enables measurements over oceans. The basic observation concept and requirements were presented in [8] and more detailed in [1]. Here, we briefly describe the two instrument designs resulting from the completed phase A/B1 studies carried out by the consortia led by Airbus Defense and Space (ADS), and OHB/Thales-Alenia. Fig. 1 depicts these instrument design concepts, in the following denoted as Concept A (left image of Fig. 1) for the design of the ADS-led consortium, and Concept B (right image of Fig. 1) for the design of the OHB-led consortium.

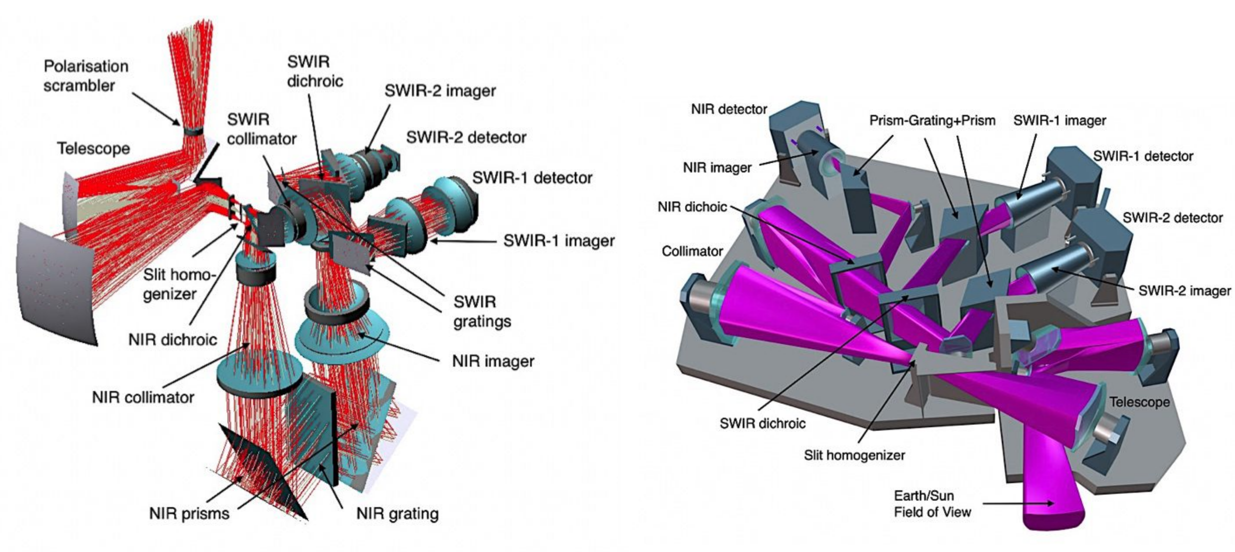

Fig. 1: Designs concepts for the CarbonSat instrument resulting from the industrial Phase A/B1 studies. Concept A on the left was developed by the consortium led by Airbus DS, Concept B on the right by OHB/Thales.

The first optical element in both designs is a polarisation scrambler for reduction of instrument's radiometric dependence on the polarisation of the incoming light. These devices are variants of a Dual-Babinet Pseudo-depolarizer (DBPD), whose principle is explained in [9]. Both concepts employ a common reflective telescope to feed the subsequent three spectrometers for the NIR, SWIR-1 and SWIR-2 bands, as well as a slit homogenizer (SH) instead of a conventional entrance slit. The purpose and designs of the SH devices is reported in Section V. Following the slit, Concept A separates the NIR band by dichroic beam split and employs two separate refractive collimators, one for the NIR band and another for the two SWIR spectrometers.
In contrast, Concept B implements a common reflective collimator, with subsequent band separation by two consecutive dichroic splitters in the collimated beam. Also the selected solutions for diffraction gratings are quite different: While Concept A deploys a transmissive plane grating in the NIR and two reflective immersed silicon gratings in the SWIR, Concept B implements transmissive prism-grating-prism assemblies made of fused silica in all three bands. The grating solutions of both concepts are based on novel technologies, which are described in more detail in Section IV. Finally, the imagers focus the dispersed light onto CCD detectors in the NIR and Mercury-Cadmium-Tellurite CMOS detectors in the two SWIR bands. Both concepts adopt a solution based on the focal plane assembly developed for the Sentinel-5 mission. The common SWIR detector technology is described in Section III.

Despite the significantly different instrument design and deployed technologies, both concepts were demonstrated to meet the challenging system requirements in terms of radiometric and spectral accuracy and stability [1]. Table 2 summarizes the main parameters and design features of the two CarbonSat concepts.

Table 2: Main characteristics of the two instrument concepts.

Telescope	Common telescope with polarisation scrambler and entrance slit homogeniser Entrance Pupil 28 mm	Entrance Pupil 29 mm
Collimator	Two refractive collimators, separate for NIR and SWIR bands	One reflective collimator, common for all bands
Band separation	Dichroic split NIR/SWIR in diverging beam, SWIR-1/SWIR-2 in collimated beam	Dichroic split NIR/SWIR and SWIR-1/SWIR-2 in collimated beam
Dispersers	Reflective immersed gratings in SWIR, binary structure transmission grating in NIR	Prism-Grating-Prism assemblies with bonded binary structure transmission grating
Imagers	Silicon, ZnSe (SWIR) and fused-silica (NIR) lenses, band-pass filters	Glass (NIR) and silicon (SWIR); band-pass filters
Detectors	Mercury-Cadmium-Telluride detectors in SWIR, CCD in NIR	

III. SWIR DETECTORS

The detectors considered for the SWIR bands are the SWIR detector array currently under development by SOFRADIR for the Sentinel-5 programme [10]. The detector is constituted of a two-dimensional HgCdTe photodiodes array that is hybridized on a Read-Out Integrated Circuit (ROIC). The two SWIR detectors are strictly identical. The Hg/Cd composition of the detection layer is tuned in order to achieve a cut-off wavelength around 2.5µm. The detector is of snapshot type, with all individual pixels integrating at the same time and the readout of the frame is performed in Integration While Read (IWR) mode. The main detector characteristics are summarized in Table 3.

Table 3: SWIR detector main characteristics

Array size (pixels)	1024 x 1024
Pitch	15 µm
Input stage	CTIA
Readout mode	Snapshot and IWR
Saturation level	Typical value 0.59 Me-
Quantum Efficiency	>85% in spectral range 400-2400 nm
RIOC noise	< 170 e^- rms @ 170 K
Reflectivity	< 3%
Total Power dissipation	< 140 mW (typical value)

IV. DIFFRACTION GRATINGS

A. Silicon immersed reflective gratings

The disperser solution for the SWIR bands selected in Concept A builds on heritage from the Sentinel-5 mission currently being implemented [9]. It is based on immersed gratings that are etched into pure silicon wafers, bonded onto monolithic silicon prisms. Silicon-immersed gratings have been developed by the Netherlands Institute for Space Research (SRON) for the Tropomi instrument of the Sentinel-5 Precursor mission [11], although Tropomi deployed monolithic silicon prisms.

The general principle of a reflective immersed grating is depicted in Fig. 2a: The incoming collimated light enters the silicon prism and is refracted towards the opposite surface with the bonded substrate. The light is diffracted by total internal reflection at the silicon-air transition of the grating structure (depicted in Fig. 2b), which is etched onto the surface of the substrate (Fig. 2b). When exiting the prism the light passes through the front surface again and is further dispersed by refraction. Such silicon-immersed gratings generate very high angular dispersion due to the diffraction inside the high-refractive index material combined with refraction at the exit surface. The latter is particularly large due to the high refractive index of silicon for SWIR radiation (~3.4). As a consequence, the size of the SWIR spectrometer is significantly reduced compared to concepts using conventional grating technology.

A key feature of the particular realization of a silicon-immersed disperser is that the grating profile etched onto the substrate surface is making use of the regular structure of the ion lattice of the high-purity silicon wafer. The manufacturing process is based on anisotropic etching in silicon, which generates facetted triangular structures on the surface of a substrate with very low roughness and highly stable period. A scanning electron microscope (SEM) image of the grating surface profile is depicted in Fig. 2c.

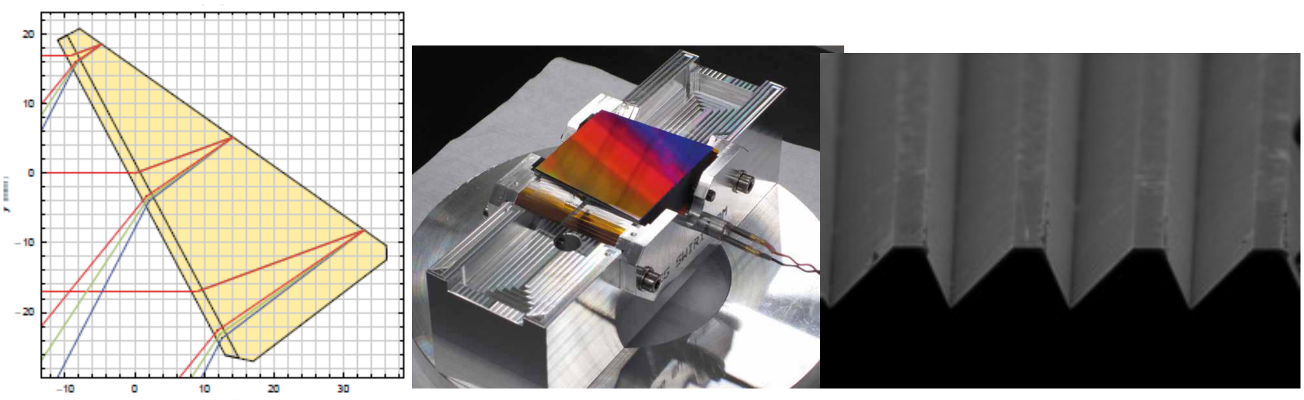

Fig. 2: a) Left: Shape and optical path of the silicon-immersed gratings developed during the CarbonSat pre-development activities. The light is dispersed by diffraction at the regular surface profile while undergoing total internal reflection at the silicon-air interface. The light is further dispersed by refraction when exiting through the front surface. b) Middle: The etched grating substrate prior to bonding to the Si prism (photo courtesy of SRON). c) Right: SEM image of the facetted triangular structures on the surface of the bonded substrate. These smooth and highly regular structures are generated by anisotropic etching into the silicon lattice.

In the course of the pre-development activities, three prototypes of the SWIR-1 grating have been manufactured and were subject to comprehensive performance testing. Due to the larger size of the prisms compared to the Sentinel-5 counterparts, the bonding of the grating substrate has proven difficult. After the first bonding processes several void areas have been detected at the prism-substrate interface with sizes on the order of a few mm^2. By optimising the bonding process, the number and size of the voids could be significantly reduced, and the impact on performance can be considered negligible. The performance tests are on-going, and the diffraction efficiency is expected to marginally meet the required 70% efficiency across the SWIR-1 wavelength range.

B. Prism-grating-prism assemblies with binary structures in fused silica

Another innovative disperser solution was devised for Concept B at the Fraunhofer Institute of Applied Optics and Precision Engineering (IOF), Germany. It makes exclusive use of fused silica as substrate material and is therefore suitable for all spectral bands of CarbonSat, including the NIR. Similar to the immersed grating, the required high spectral dispersion is reached by a combination of diffraction with refraction. This is reached by an assembly comprised of a prism with a grating substrate optically bonded onto its exit surface. Separated by an air-gap follows a second prism, which is shaped to correct for smile distortion of the dispersed light. The principle of these prism-grating-prism (PG+P) assemblies is depicted in Fig. 3a: The collimated light passes through the first prism with the grating substrate bonded on its exit surface. The dispersed light enters the second prism, and the PG+P assembly effectively acts as an immersed grating enhancing the angular dispersion. The prism angles are optimised for correcting keystone and smile distortions. Although PG+P assemblies are used in all three spectrometers of Concept B, the different spectral requirements give rise to very different grating parameters and coatings.

The key technology of this grating solution is the generation of a special grating profile based on photonic sub-micron structures. An effective-medium grating is created by etching a binary step structure of sub-wavelength dimensions into the surface of a fused-silica substrate. Fig. 4b shows such structures, which are generated by an electron-beam lithography process in combination with reactive-ion etching. The trenches and bars of the binary structure are covered by a conformal titanium dioxide over-coating applied by atomic layer deposition. These binary transmission gratings are operated in Littrow configuration and are characterised by very high diffraction efficiency and low polarisation sensitivity, as shown in Fig. 4.

In the course of the breadboard study, several test samples and full size gratings for the NIR and SWIR-1 PG+P assemblies have been manufactured and tested. The design and manufacture of the NIR grating proved to be particularly challenging. The high spectral resolution required in this band (0.1 nm) translates into a high grating frequency on the order of 2000 lines per millimetre and deep grating profiles with high aspect ratio (trench depth-to-width ratio) of about 7.

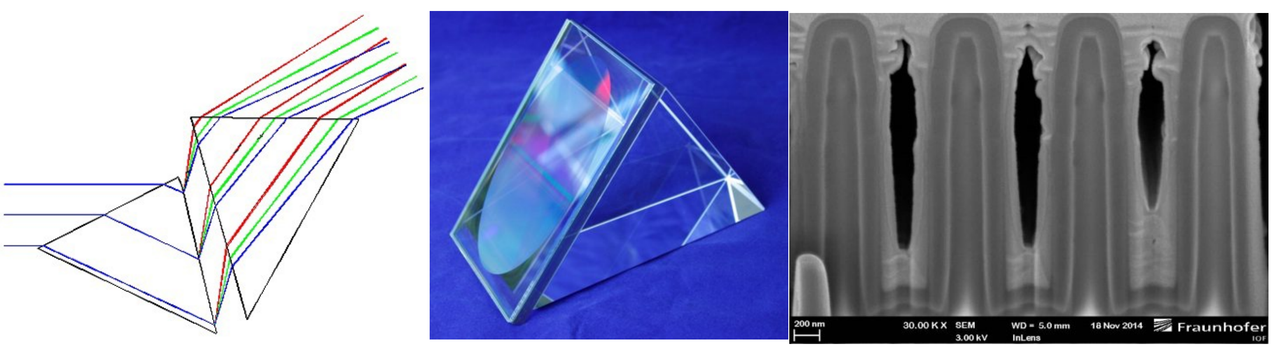

Fig. 3: a) Left: Light path though the prism-grating-prism (PG+P) assembly. b) Middle: The bonded prism grating prototype assembly (photo courtesy of IOF). c) Right: SEM image of the binary sub-micron structure on the surface of the grating substrate.

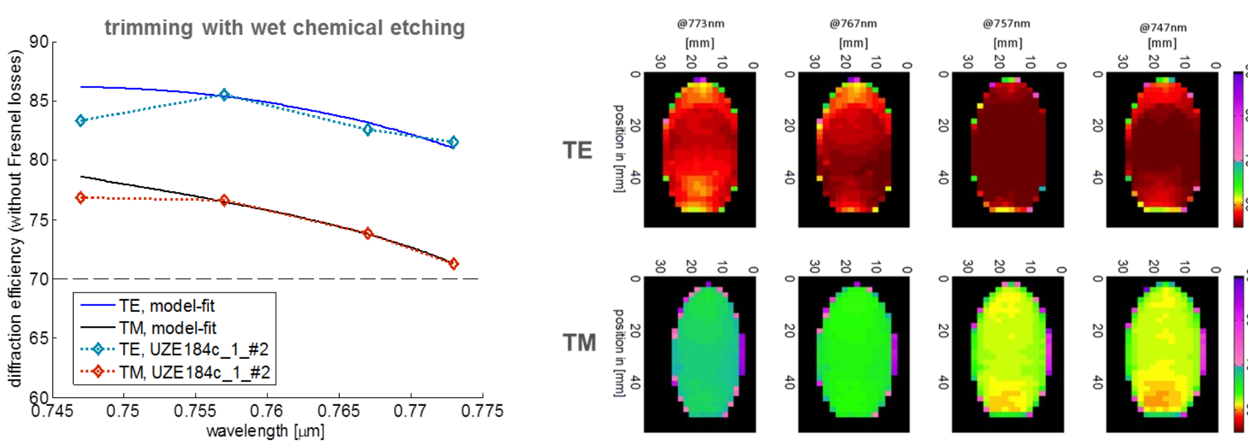

Fig. 4: a) Left: Predicted and measured diffraction efficiency of a NIR PG+P grating for two polarization directions. The resulting poslarisation sensitivity is below 7%. b) Right: Homogeneity of efficiency across the pupil

V. SLIT HOMOGENISERS

A push-broom imaging spectrometer images the ground scene directly onto the entrance slit. The natural inhomogeneity of Earth reflectance (e.g. due to albedo contrast and clouds) results in non-uniform and highly variable illumination of the entrance slit. As a consequence, the image of a conventional entrance slit changes rapidly as the field-of-view is scanning the ground scene, distorting the Instrument Spectral Response Function (ISRF) in an unpredictable manner. The magnitude of the ISRF distortion depends on the ratio between the size of the slit projection and the spatial sampling distance in ALT direction. For CarbonSat, with about 500 m projected slit width on the ground and 2 km SSD along the track, the effect turns out to be critical. Simulations of this effect over reference scenes predict ISRF distortions >10%, which is not compatible with the stringent requirement (<2%).

In order to reduce radiometric errors resulting from inhomogeneous illumination at the slit entrance, both consortia have designed so-called slit homogenizers (SH), whose general setup is shown in Fig. 5a. These devices can be understood as entrance slits comprised of two parallel mirrors, which act as waveguides along the optical axis. As the light beam propagates along the SH, it is reflected multiple times by the mirrors. These reflections and coherent interference of the wavefronts result in a re-distribution of energy across the SH width, which effectively scrambles the radiometric non-uniformity. The principle of a SH is described in more detail in [12].

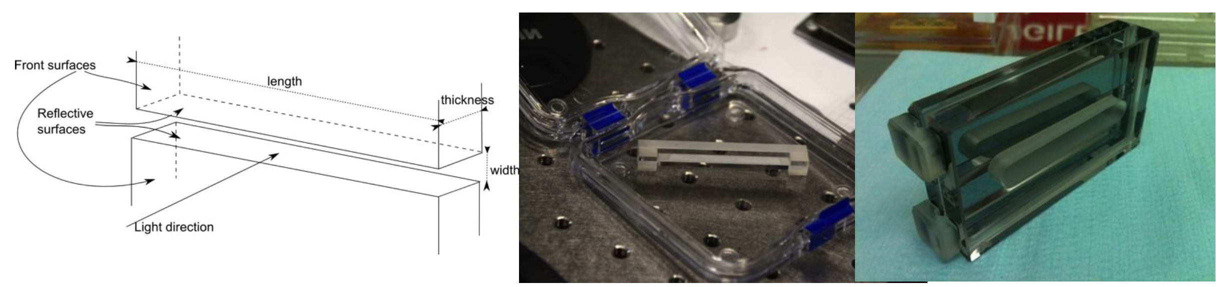

Fig. 5: a) Left: General setup of a slit homogenizer (SH). b) Middle: SH prototype for Concept A (photo courtesy of Airbus DS) c) Right: SH prototype for Concept B (photo courtesy of WinLight)

Fig. 5b and 5c show the devices manufactured by each consortium during the breadboard studies. The SH prototype developed for Concept A (Fig. 5b) consists of two Zerodur plates, which are coated with aluminium and protective SiO_2. The plates are separated by 107 µm defining the slit width, and form a structure with 50 mm slit depth along the optical axis. For Concept B WinLight Systems developed a flight-representative SH device with all components made of fused silica (see Fig. 5c). The mirror coating on the inner reflecting surfaces, separated by 118 µm, is silver with a 100 nm protective layer. The breadboard was mechanically tested and found to meet the stringent requirements and tight tolerances.

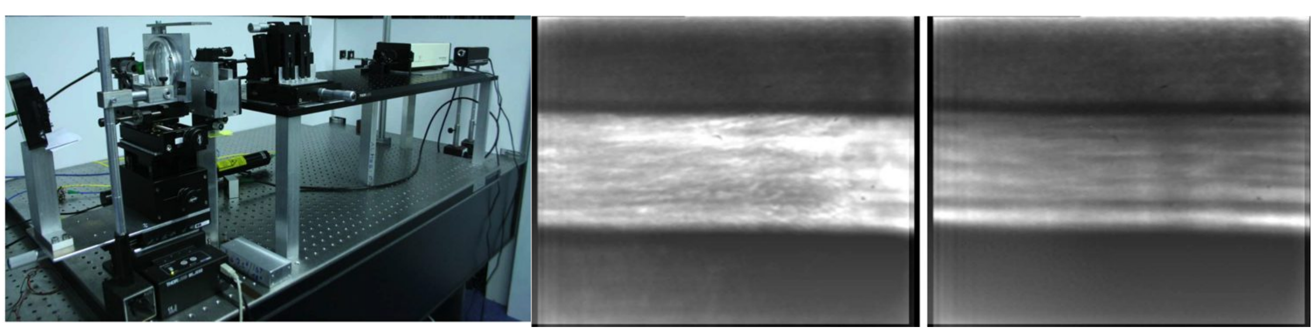

Fig. 6: a) Left: Test setup for SH performance testing (photo courtesy of ITO). b) Middle: SH response (image of slit exit) to homogeneous illumination. c) Right: SH response to half-slit (knife-edge) illumination.

While geometric optics would predict perfect scrambling performance, in real devices interference between reflected beams will alter the intensity distribution at the exit of the SH. Model simulations of resulting interference patterns predict sufficient scrambling performance for SH devices with depths of a few mm, and at some point cannot be further improved by more reflections with larger depths. In order to test the predictions, the SH device of Concept A has been characterised at the Institute of Technical Optics (ITO), University of Stuttgart, Germany, in terms of its response to various non-uniform intensity patterns. As an example, Fig 7 shows a measured image of the intensity distribution at the SH exit, in response to a half-slit illumination at the entrance (one half of slit entrance blocked in slit width dimension). The figure shows that the radiation is effectively re-distributed across the slit exit. The superimposed intensity variations also occurred for a homogeneous input illumination, and are in large part attributed to residual speckle patterns of the laser source used as input stimulus. While the current results confirm the functionality of SH devices, the test setup at ITO will be further refined for future characterisations.

VI. SUN DIFFUSERS

Besides the pre-development activities presented above, both CarbonSat consortia have thoroughly investigated the use of Sun diffusers for in-flight radiometric calibration. While the use of the Sun as calibration source is standard for atmospheric chemistry missions, measurements of solar irradiance exhibit spectral features at high resolution due to speckle patterns generated by the diffuser [13]. These radiometric artifacts propagate into the observed reflectance, and represent a major contributor to the particularly challenging relative radiometric error budget. The magnitude and spectral structure of diffuser speckles depends on observation geometry, diffuser type and dimension, as well as spectral resolving power. As a consequence, resulting spectral features are difficult to predict, especially in the SWIR bands.

Both consortia have developed comprehensive models for simulating diffuser speckles and initiated laboratory tests for their validation. For Concept A a model combining ray-tracing with wave propagation was developed (by Scoptique, France) and applied to volume diffuser materials (OM-100 by Heraeus) as well as a Quasi-Volume-Diffuser (QVD). Hardware tests are envisaged to verify the model calculations. For Concept B, Insititute d'Optique Graduate School (IOGS), Paris, France, developed a rigorous semi-empirical model to simulate the propagation of speckle patterns from the telescope focal plane to the spectrometer focal plane, and their polarisation, angular and spectral averaging. A measurement campaign was performed to thoroughly characterised Spectralon diffusers and the obtained parameters (polarization behavior, angular de-correlation and spectral de-correlation) were inserted in the model. This activity, which can be extended to other diffuser types, will be presented in a separate paper.

VII. CONCLUSIONS

The CarbonSat industrial studies in the frame of the eighth Earth Explorer activities were accompanied by a comprehensive pre-development programme for critical components. In this paper we presented the results for breadboard activities, and their relation to the requirements of the mission. The prototype developments for diffraction gratings and slit homogenizers were shown and first laboratory test results presented. We also briefly reported on hardware and model simulation developments to quantify spectral features introduced by Sun diffuser. The test results indicate that the particularly stringent requirements for precise measurements of greenhouse gas concentrations can be met with deployment of dedicated components developed during the CarbonSat instrument studies.

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