Compressive sensing of trace gases: replacing diffractive elements by nanostructured transmission filters on a detector

Executive summary report of ESA Open Space and Innovation Platform study

Prepared by:	Ralf Kohlhaas	Ralf Kohlhaas Digitally signed by Ralf Kohlhaas Date: 2023.03.17 14:56:19 +01'00'
	Marijn Siemons	Marijn Siemons Digitally signed by Marijn Siemons Date: 2023.03.17 14:48:31 +01'00'

Document Change Record

Issue	Date	Changed Section	Description of Change
1	17 March 2023	All	Initial version

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Reference Documents

[RD1] Marijn Siemons and Ralf Kohlhaas. *Final technical report of Compressive sensing of trace gases: replacing diffractive elements by nanostructured transmission filters on a detector*. SRON-CSPEC-RP-2023-001 issue 1. Mar. 2023.

[RD2] Zhu Wang et al. "Single-shot on-chip spectral sensors based on photonic crystal slabs". In: *Nature Communications* 10.1 (Mar. 2019). DOI: 10.1038/s41467-019-08994-5.

1 Introduction

Climate change is a threat to the health and lives of humans and of the biodiversity of this planet. To properly estimate the effects and sources of anthropogenic climate change, both models and independent observations are needed. The independent observations should have a high spatial and temporal resolution and be as precise and accurate as possible. A high spatial and temporal resolution are especially important for identifying sources of greenhouse gases. This can be used to directly approach the responsible parties of polluting sites. This is for example the goal of the Methane Alert and Response System (MARS). Precise and accurate measurements are needed as input to the climate models to reduce uncertainties in their predictions. This can increase the political pressure to take countermeasures. Independent observations of the planet can be achieved over satellite missions with an open data policy. A very successful example in this direction is the Copernicus Programme of the European Commission/European Space Agency with its Sentinel satellites. The main measurement instrument type used in these satellite missions are grating imaging spectrometers. At the heart of those instrument are gratings which split incident light in different colors or spectral components which can then be recorded on a detector. In case of an earth observing satellite, the incident light is the sun light which is reflected from the earth and collected by the telescope of the satellite instrument. From the fingerprint of the measured spectrum the abundancy of different gases in the atmosphere or the composition of the ground can be inferred. Earth observing satellite instruments using this principle have led to considerable advances in the understanding of this planet. A natural question to ask is if novel types of instruments and observation strategies could push our knowledge even further.

2 Beyond Imaging Grating Spectrometers

Grating spectrometers reach back in history to the 17th century and have been perfected for satellite missions with recent innovations such as slit homogenizers and ultra-low stray light gratings. They are the reliable workhorse which will continue to support earth observation missions in the future. However, grating spectrometers are intrinsically not the most efficient solution for building instruments to measure the planet. Any passive optical measurement instrument should try in its design to maximize the Signal-to-Noise Ratio (SNR) and to adapt the measurement basis to the target signal while minimizing the instrument volume. Imaging grating spectrometers for earth observation do not fulfill this to a full extent because of:

- A limited along-track (ALT) measurement swath which is needed for the grating operation, resulting in the collection of less light than in principle possible.
- Recording of a complete spectrum in a spectral range, while only parts of the spectrum contain relevant information on the target gas or ground to be measured.
- Free space optical path length needed for spectral dispersion.

Still, due to the success of grating spectrometers and the effort of their optimization for earth observation, it is very difficult to find a solution which considerably improves upon their performance. A possible route to take here is to resort to novel technologies and algorithms. The main components of this study were the use of photonic crystals and of compressive sensing. Their combination shall improve earth observing satellite instruments in the following ways:

- Expansion of the ALT swath to approximately the size of the across-track (ACT), therefore significantly increasing the SNR.
- Choice of the measurement basis (photonic crystal transmission functions) adapted to the measurement target at hand, optimized together with the retrieval algorithm.
- Spectral diversity folded into the photonic crystal response, eliminating the need for free space optical distance for spectral dispersion.

The technical results have been given in the final report [RD1] of the project and in the following a few key concepts and results are summarized.

3 Photonic Crystals and Compressive Sensing

A novel component for earth observation used in this study are photonic crystals. These are artificial structures made of dielectric materials (such as silicon or silicon nitride) with periodic changes in the refractive index. We use here 2D photonic crystals which are manufactured in this project by etching periodic holes or other periodic structures in a thin layer of silicon. Photonic crystals show very similar effects in the confinement of light as for electrons in periodic crystals in solid state physics. In the same way as in solids, bands of allowed energy eigenstates and gaps exist. This is exploited in this project by working in a regime where the photonic crystals have transmission spectra with a quasi-random functional response as a function of wavelength. With a large available library of different transmission functions the best set can be chosen to measure for example a specific trace gas. Compressive sensing breaks with the rule that there always needs to be at least as many equations as variables in a system of equations to be able to solve it. This can be done if there is other available information known about the system which can help to find a solution. In compressive sensing, this is done by converting the system of equations to a different representation, or basis, where the variables or equivalently the signal to be retrieved is known from the onset to be sparse. This means only a few variables are needed to represent the signal in this basis. Since gasses in the atmosphere have molecular structures with known transition frequencies, this prior knowledge can be used to design a basis where compressive sensing is possible. This means that less filters than target spectral points can be used to reconstruct a spectrum. From that a gas abundancy can be measured in an efficient way.

4 Instrument Concept

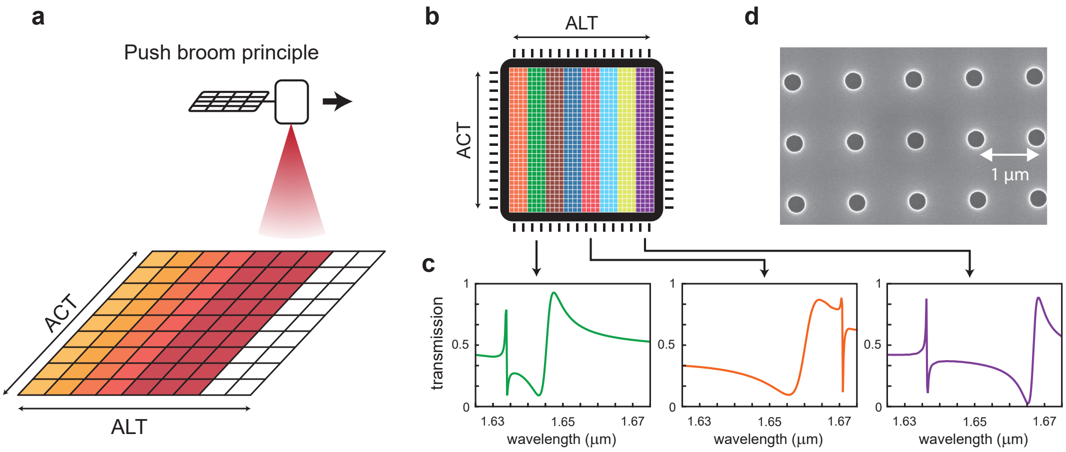

Figure 1: Principle of photonic crystal satellite instrument.

The instrument concept consists of the idea to have an array of photonic crystal filters directly attached to a detector and to fly with a satellite instrument in low earth orbit over the ground. In the along-flight direction filters with different hole patterns and therefore transmission functions are arranged. The number of different filter shapes will be at least three times lower than the number of detector ALT pixels. In the perpendicular ACT direction, the same filter shapes are used on the detector for the same ALT detector position, leading to a stripe pattern on the detector. When the satellite flies over the ground, different filter functions one after each other scan over the scene. Each pixel measures only a constant signal value, but from the knowledge of the transmission functions a spectrum can be reconstructed. This is then used for example for a gas retrieval. General spectrometers based on photonic crystals in the visible have been invented recently [RD2] and were a trigger for this study. The main novelty of this project consisted in the transfer of the concept to earth observation and integration in an instrument concept specialized for the detection of a specific target gasses from a moving satellite platform.

5 Results

As a target for this study the detection of methane was chosen due to the equipment for testing readily available at SRON and the availability of classical reference instrument designs for performance comparisons. First photonic crystal samples were manufactured and measured and compared to simulations. A large library of simulated photonic crystals was generated and the compressive sensing algorithm dedicated for this measurement problem was developed. An efficient basis for the spectrum reconstruction and compressive sensing could be found, but it still showed biases in the methane retrievals. Further investigation showed that a direct retrieval method over the filter functions had the best performance in terms of precision and accuracy. A further interesting development during the project was that a group at the Leiden Institute of Advanced Computer Science applied their evolutionary algorithm for the filter selection, which gave the best results over other investigated methods.

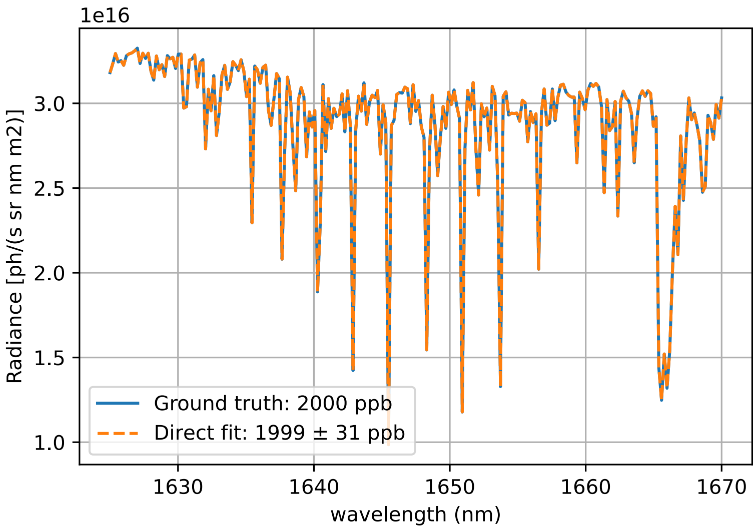

Figure 2: Reconstructed spectrum from photonic crystal filter measurements and comparison to original methane spectrum.

Based on the results in this study, a first instrument concept with the main parameters summarized in table 1 was set up. For the low radicance reference scenes and albedo of 0.15 and a solar zenith angle of 70 degrees was assumed and for the high reference scenes an albedo of 0.7 and solar zenith angle of 10 degrees. No forward motion compensation (stare mode) was assumed.
The instrument concept shows a comparable performance to a classical grating spectrometer currently under development, but with a more than 10 times lower aperture area. The clear reduction in system size for the same performance motivates further experimental and theoretical investigations into the instrument concept. Main performance improvements could be especially achieved by finding photonic crystals which preserve as much as possible a diverse transmission spectrum under a large angular range of incidence.

Detector Material	InGaAs
Format (ALT x ACT)	640 x 512
Pixel size b_{pix} [μm]	15
Entrance aperture dimensions a_{ALT} x a_{ACT} [mm^2]	18 x 18
Ground resolution element size ALT x ACT [m^2]	300 x 300
Spatial sampling distance ALT x ACT [m^2]	50 x 60
F-number F_{ALT} x F_{ALT}	8.3 x 7
Swath ALT x ACT [km^2]	32 x 30
Number of photonic crystal filters	16
Methane precision for low radiance scenes [%]	1.4
Methane precision $\sigma_{\text{CH4,high}}$ [%]	0.4

Table 1: Main instrument and performance parameters of first photonic crystal instrument design.