Document Version
Final published version

Citation (APA)
Bui, K., Falckenheiner, S. I., Piron, P., Kooi, B. J., & Gerini, G. (2025). Reconfigurable Sb_2Se_3 metasurface filter design for compressive-sensing-enabled atmospheric trace-gas recognition. In *19th International Congress on Artificial Materials for Novel Wave Phenomena, Metamaterials 2025* (pp. X108-X110). (19th International Congress on Artificial Materials for Novel Wave Phenomena, Metamaterials 2025). IEEE. https://doi.org/10.1109/Metamaterials65622.2025.11174214

2025 Nineteenth International Congress on Artificial Materials for Novel Wave Phenomena (Metamaterials) | 979-8-3315-3656-5/25/$31.00 ©2025 IEEE | DOI: 10.1109/Metamaterials65622.2025.11174214

19^{th} International Congress on Artificial Materials for Novel Wave Phenomena - Metamaterials 2025
Amsterdam, The Netherlands, Sep. 1^{st} - 6^{th} 2025

Reconfigurable Sb_2Se_3 metasurface filter design for compressive-sensing-enabled atmospheric trace-gas recognition

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Abstract – **In this paper, we propose the design of a reconfigurable metasurface filter incorporating phase change materials (PCMs). This filter is part of a novel spaceborne spectrometer concept for atmospheric monitoring. The metasurface filter consists of PCMs pillars embedded in a diamond matrix. The combination of shape and material properties results in resonances that give rise to specific spectral filtering functions. The optical properties of PCMs, and hence the transmission function, change when stimulated with a pulsed laser. In combination with a compressive sensing (CS) algorithm, a limited number of measurements with a single metasurface results in precise reconstructions of the Earth's atmospheric spectrum.**

I. INTRODUCTION

Decision-making in climate-action requires monitoring anthropogenic atmospheric trace gases. This is generally done with high-resolution spaceborne spectrometers, which tend to be bulky. Reconfigurable metasurfaces are a promising technology to miniaturise spectrometers, when used in combination with compressive sensing (CS). This sensing technique takes advantage of the sparsity of the signal in a chosen basis, and the incoherence of the measurements to reconstruct the original signal [1], which in this case is the spectrum. The reconfigurability of the metasurface is achieved through the use of phase change materials (PCMs). Previous works have proposed the combination of these three elements (metasurfaces, CS, and PCMs) for imaging [2] and on-chip spectroscopy [3]. In this work, we propose a design methodology for a metasurface filter using PCMs for the detection of CH_4 and CO_2 in the short-wave infrared (SWIR) band between $1585\,\mathrm{nm}$ and $1680\,\mathrm{nm}$ using CS. The novelty of this work lies in the use of this combination for remote sensing. The filter operates in transmission, and can be readily integrated into the optical chain of a compact instrument for trace gas recognition in the context of an Earth observation mission.

II. WORKING PRINCIPLE

The proposed instrument concept performs a sequence of N measurements of the incoming light in a time multiplexing scheme. The different measurements are performed through a reconfigurable metasurface filter exploiting N different crystallinity states of the PCM nano-resonators. These measurements are used as input to the CS algorithm for the spectral reconstruction. This concept is presented in Fig. 1, where measurements I_i and transmission functions T_i at times t_i with $i \in [1, N]$ are used to reconstruct the spectrum $s(\lambda)$ as a function of wavelength λ. A detailed discussion of the CS algorithm can be found in [4]. Cloud properties such as trace-gas concentrations and altitude can then be inferred from the reconstructed spectrum with inverse modelling or other retrieval algorithms.

Sb_2Se_3 has been chosen as the PCM because of its large refractive index contrast of approximately 0.7 between its amorphous and crystalline states [5]. This decreases the correlation between transmission functions, and hence measurements, of different crystallinity states. Furthermore, its negligible absorption in the SWIR band increases the signal-to-noise ratio of the measurements.

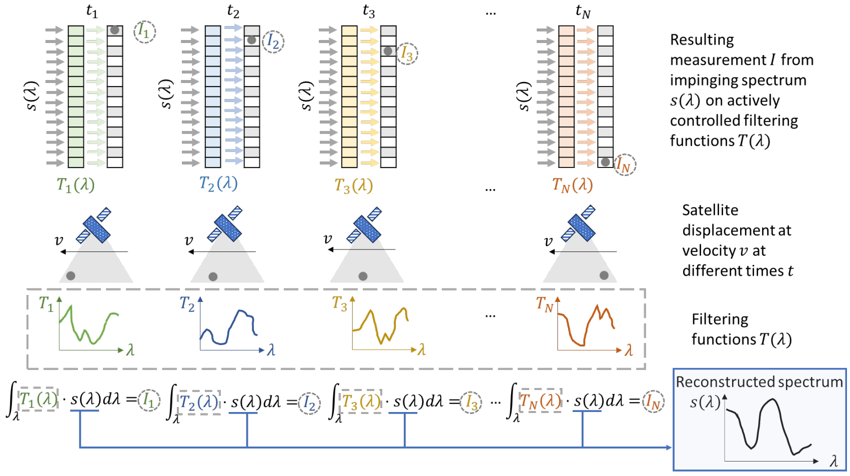

Fig. 1: Time-multiplexed measurement concept for Earth observation.

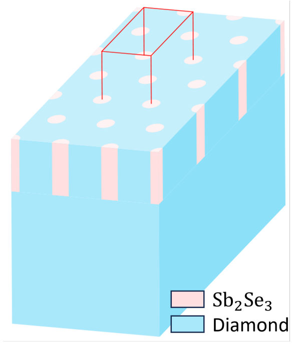

Fig. 2: Metasurface 3D view.

An increase in the PCM temperature is needed to change the crystallisation. This is achieved with a pulsed laser centred around 360 nm, where Sb_2Se_3 has a high absorption [5]. Sb_2Se_3 crystallises when applying a low energy pulse in the order microseconds and reverts completely to amorphous when applying a high-energy pulse in the order of femtoseconds, followed by rapid cooling to avoid crystallisation [6]. A matrix surrounding the PCM is needed to hold the PCM in place during the melt-quenching process. Diamond was chosen because it has a high thermal conductivity, which facilitates melt-quenching the crystalline into the amorphous state, and it exhibits negligible losses in the SWIR band. Currently, 6 states have been demonstrated for 65 nm Sb_2Se_3 films [7], but it is expected that for larger Sb_2Se_3 volumes, 11 states, as achieved for the PCM GeSbTe [8], may be possible. The time of an entire cycle with 11 partial crystallinity states is orders of magnitude shorter than the time an object is in the image plane of the flying platform from Fig. 1, assuming an altitude of 500 km and a swath width of 30 km.

III. OPTIMISATION AND RESULTS

To enhance reconstruction performance, transmission functions can be optimised by changing the metasurface design. To simplify the optimisation, several design parameters were fixed. First, cylindrical Sb_2Se_3 nanopillars were chosen because of their fabrication simplicity, while maintaining transmission functions with sharp resonances. Next, a hexagonal lattice was adopted because of its low polarisation sensitivity. A 3D sketch of a section of the resulting periodic metasurface and the corresponding unit cell (red box) is shown in Fig. 2. The design constraints of the unit cell, summarised in Tab. 1, are established considering suppression of diffraction orders, manufacturing constraints, and the speed at which the melt-quenching process must occur for PCM amorphisation.

The optimisation problem is shown in (1), where bold characters are vectors containing values at different wavelengths. T_a and T_c represent the transmission functions for the amorphous and crystalline states, $\bar{\mathbf{T}}_a$ and $\bar{\mathbf{T}}_c$ their average values, $\mathrm{ran}(\cdot)$ is the difference between the maximum and minimum elements of the analyzed vector, and M denotes the number of spectral points used in the simulation. The square root term is the average Euclidean distance between the crystalline and amorphous states, which represents the variation between the transmission functions of different PCM states. The second and third terms represent the spectral variation within a transmission function. The fourth and fifth terms give preference to functions with a higher transmission value.

$$\min_{D,H,\Lambda}\left[-\sqrt{\frac{1}{M}\sum_{i=1}^{M}\left|T_a(\lambda_i)-T_c(\lambda_i)\right|^2}-\mathrm{ran}(\mathbf{T}_a)-\mathrm{ran}(\mathbf{T}_c)+\left|\bar{\mathbf{T}}_a-0.7\right|+\left|\bar{\mathbf{T}}_c-0.7\right|\right] \tag{1}$$

The metric between the brackets in (1) was chosen for several reasons. First, only evaluating the crystalline and amorphous transmission functions in the optimisation reduces the computation time. Second, it does not require the use of the CS algorithm, but has a higher correlation with the reconstruction error using CS compared to other evaluated candidates. For the optimisation and the electromagnetic simulation, the generational particle

Parameter	Lower bound	Upper bound
Pillar diameter D	200 nm	400 nm
Pillar height H	100 nm	1200 nm
Lattice constant Λ	700 nm	1400 nm

Table 1: Design constraints of metasurface filter.

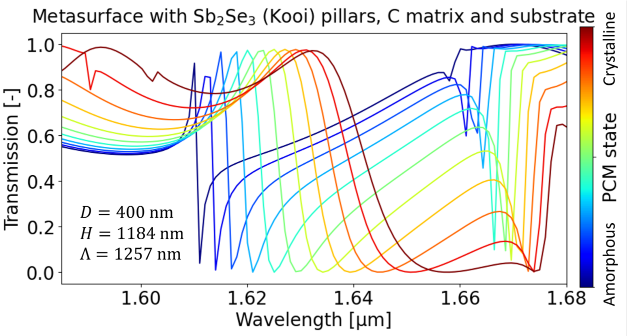

Fig. 3: Resulting transmission functions.

swarm optimisation algorithm and the rigorous coupled-wave analysis implementation of the ANSYS® Lumerical Inc. STACK solver (release 2024 R1) were used. The optimised transmission functions and the corresponding design parameters are shown in Fig. 3, where each transmission function has multiple resonant peaks and dips to facilitate the spectral reconstruction using CS. This result was used for the reconstruction of a verification set of atmospheric spectra containing different concentrations of trace gases, resulting in a mean reconstruction error that is three orders of magnitude below unity. The use of the optimised transmission functions in the CS reconstruction process is discussed in [4].

IV. CONCLUSION

In this paper, we have presented the working principle of an actively controlled metasurface filter with PCM nanopillars, used for trace gas recognition in a spaceborne Earth observation mission. The design methodology of the filter is discussed, which resulted in a design optimised for atmospheric spectrum reconstruction using CS.

ACKNOWLEDGEMENT

This publication is part of the project NL-ECO: Netherlands Initiative for Energy-Efficient Computing (with project number NWA. 1389.20.140) of the NWA research programme Research Along Routes by Consortia which is financed by the Dutch Research Council (NWO). For the purpose of open access, a CC BY public copyright licence is applied to any Author Accepted Manuscript version arising from this submission.

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