

# Pixelated Resonant Subwavelength Grating Filters for Greenhouse Gas Monitoring

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## ABSTRACT

We describe the design of pixelated filter arrays for hyperspectral monitoring of CO<sub>2</sub> and H<sub>2</sub>O absorption in the midwave infrared (centered at 4.25 $\mu$ m and 5.15 $\mu$ m, respectively) using resonant subwavelength gratings (RSGs), also called guided-mode resonant filters (GMRFs). For each gas, a hyperspectral filter array of very narrowband filters is designed that spans the absorption band on a single substrate. A pixelated geometry allows for direct registration of filter pixels to focal plane array (FPA) sensor pixels and for non-scanning data collection. The design process for narrowband, low-sideband reflective and transmissive filters within fabrication limitations will be discussed.

**Keywords:** grating, subwavelength, pixelated, filter, sensor, hyperspectral

## 1. INTRODUCTION

We design filters for an optical micro-sensor capable of quantifying the concentrations of greenhouse gasses in localized regions of the atmosphere. This sensor is a pixelated, hyperspectral arrayed optical component integrated with a focal plane array (FPA). The key optical component is a pixelated hyperspectral filter array. Filters with exquisite wavelength control are made possible by utilizing tailored resonant subwavelength gratings (RSGs) in the place of traditional multi-layer thin-film stacks.

The differentiating technology is an integrated RSG whose nanostructure can be geometrically scaled to access a wide center-wavelength range and maintain a very narrow waveband (0.1-10nm). The configuration of the RSG is an all-dielectric device that selectively reflects a wavelength of interest while transmitting the majority of the beam for further measurement. With an arrayed approach, highly-resolved data may be accumulated with a non-scanning, "snapshot" system. We present both reflecting and transmissive filter designs using the RSG structure.

### 1.1 Water and Carbon Dioxide Bands

We currently have considerable absorption data from satellites in the longwave infrared (LWIR, 8-12 $\mu$ m). However, these absorption spectra are spatially low-resolution and integrated through the entire atmosphere. With a local sensor, we can address effects associated with a population or region of a country and more fully understand changes of concentrations with altitude. This locally attributed information is necessary to accurately pinpoint climate changing cause and effect. Perhaps more importantly, the role of water vapor and clouds can be characterized with such data. Water vapor participation in the greenhouse effect is not well understood and may be the most significant in the process as it varies with temperature and altitude, and is the only greenhouse gas that also exists in liquid and solid phases. Our proposed technology differs from satellite-based sensors that integrate over the entire atmosphere. Local measurement, though difficult, allows a more accurate depiction of water and gas distributions across heights in the column of air extending from sea level to the upper atmosphere.

The monitoring wavelength range that we utilize encompasses the midwave infrared (MWIR, 4-8 $\mu$ m) atmospheric waterbands and CO<sub>2</sub> absorption bands, so that we can sensitively (on the order of 1m distances) monitor water vapor, clouds, and CO<sub>2</sub> as a function of altitude. Whereas this spectral region is often avoided due to its high absorption over long distances, the high absorption is actually an asset for local monitoring with a relatively compact system. Here significant, but not total, absorption occurs over short distances. A sample measured absorption spectra of water vapor and CO<sub>2</sub> through 1m of atmosphere can be seen in Figure 1. The richness of the absorption spectra is evident. We will focus our efforts on the CO<sub>2</sub> and H<sub>2</sub>O absorption bands labeled (2) and (3) in Figure 1.

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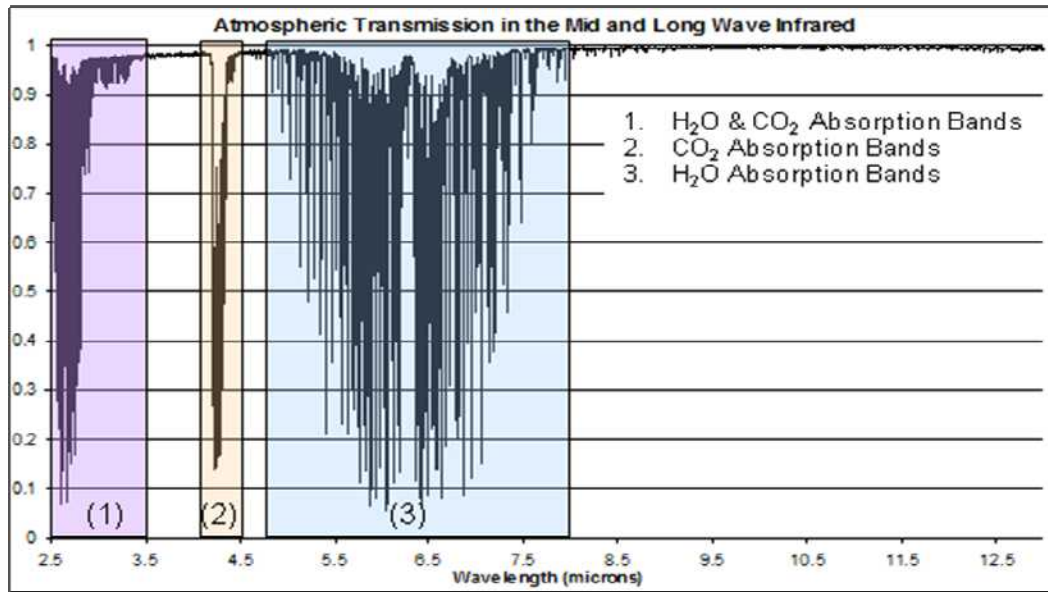


Figure 1. Measured atmospheric transmission through 1 meter of air using a Fourier transform infrared spectrometer (FTIR).

## 1.2 Resonant Subwavelength Gratings

Resonant subwavelength gratings (RSGs) have been studied considerably. [1-3] The resonant conditions of the passive, all-dielectric RSG predict 100% reflection and 0% transmission at the design wavelength. This is not an approximation, but a direct consequence of using non-absorbing dielectric materials in the component. Careful design leads to very low sidebands away from resonance as seen in a sample RSG response at left in Figure 2.

The challenge of this particular measurement is the wide total band and the narrowness of the absorption features as seen in Figure 1. In the MWIR range, transparent dielectrics such as Si and Ge have a large index contrast with air, allowing for narrowband RSGs. Furthermore, they have low loss across the MWIR. Zinc sulfide offers a lower-index low-loss material to complement the high index Ge, and we use it for the multiple purposes of a reliable substrate, the low-index layer of a mirror stack in the transmissive design, and for a cover layer to reduce off-resonance sidebands. A very narrow passband, while also maintaining very good out-of-band rejection, is a necessity for a detector signal with high dynamic range, rather than a small signal on a large dc background.

Perhaps most importantly, the grating period can be changed abruptly from one RSG pixel to the next, with no dead space and 100% fill factor to realize an RSG array. Thus a dense array of RSG elements can span the entire absorption bands of H<sub>2</sub>O or CO<sub>2</sub>. We can choose the overall accessible sensing range of the linear response by adjusting the RSG fabrication parameters, such as the grating period and duty cycle, the grating and waveguide thicknesses, and the grating and waveguide materials. A linear response can be seen in the plot at right in Figure 2. The pixelated nature of these RSGs leads to questions of the effect of finite size, which have been previously discussed in [4].

Here we will describe two filter designs that utilize the RSG configuration. One is a simple reflective RSG. In the second design the RSG is combined with a thin-film stack to form a Fabry Perot cavity filter. The RSG in both designs allow us to independently select the center wavelength of each pixel filter by only changing the lithographically determined period of the grating of each pixel element. Pixelated filters need not be adjacent or in wavelength-order, since each filter's center wavelength is determined by grating pitch – pixel placement within the array can be arbitrary.

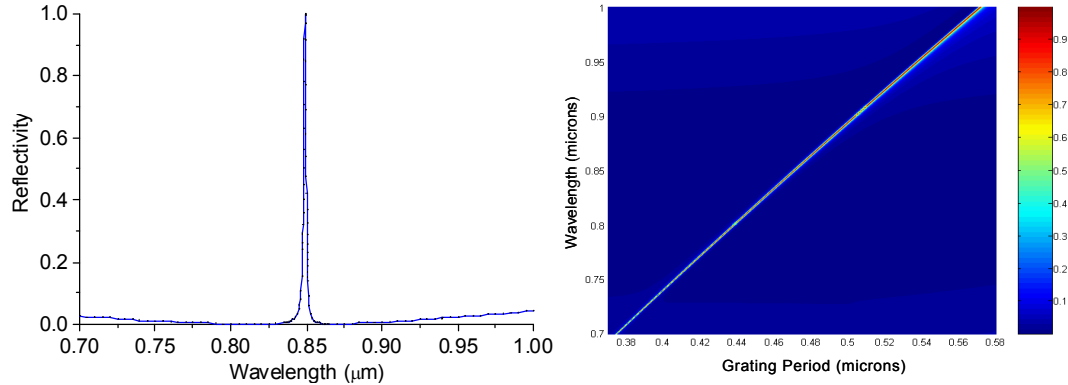


Figure 2. (left) Reflected signal from a typical RSG. Note low sidebands over an extended range and narrow reflection peak. (right) The resonance response can be seen to vary in wavelength linearly with change in grating period.

## 2. LIMITATIONS OF CURRENT TECHNOLOGIES

### 2.1 Existing Measurement Methodologies

A number of existing instruments monitor climate effects. A pyrgeometer integrates across a huge wavelength range (4.5-100 $\mu\text{m}$ ) that quantifies the exchange of IR radiation between the earth and the atmosphere for long-term climate predictions. NOAA recognizes the strong role water plays within the climate scenario and has an extensive network of antennae to monitor the total water vapor content through the entire atmosphere. Each of these commonly utilized instruments produces an integrated signal across the full solar spectrum and atmosphere; neither can characterize a differential, localized effect that is necessary for regional or population attribution.

### 2.2 Existing Filter Technologies

A filtering strategy that is often proposed is the matched filter. In this case, the measured atmospheric absorption spectrum would be convolved with the sought gaseous absorption spectrum. The desired result should be a large, narrow peak when there is a match. However, because water is a complicated multitude of very narrow peaks across a wide wavelength range, the resulting convolution of the transmitted signal will be ambiguous. As an example of the problems associated with matched filters for signals of this type we look at three absorption spectra: two water-like spectra and that of water. Figure 3a and Figure 3b are spectra representing random water-like peaks, denoted by Chemical X and Chemical Y. Figure 3c is a measured water spectra. Figure 3d-f are the resulting convolutions of a-c with the water spectra. No difference is immediately detectable, indicating that the presence of water is not definitive. The nature of the transmitted signal, near unity with a complex set of narrow absorption lines, along with the integral nature of the convolution, does not lend itself well to this methodology.

An alternate method for measuring the spectra would be to use a hyperspectral filter to measure individual wavelengths across the absorption bands. As a result of the narrow absorption lines, the individual filters in the array should also be narrowband, on the order of 1nm. One method for realizing these narrow filter bandwidths is to use a thin-film filter. However, the fabrication challenges involved with a pixelated design using traditional thin films is considerable. A serial approach where each filter pixel is layered in isolation while neighboring filter pixels are masked off makes this technology low yield, particularly for large pixel counts and with the many layers required for these narrowband filters. Compounded misalignments and rounded topologies would significantly reduce the clear aperture of each pixel and drastically impact successful fabrication.

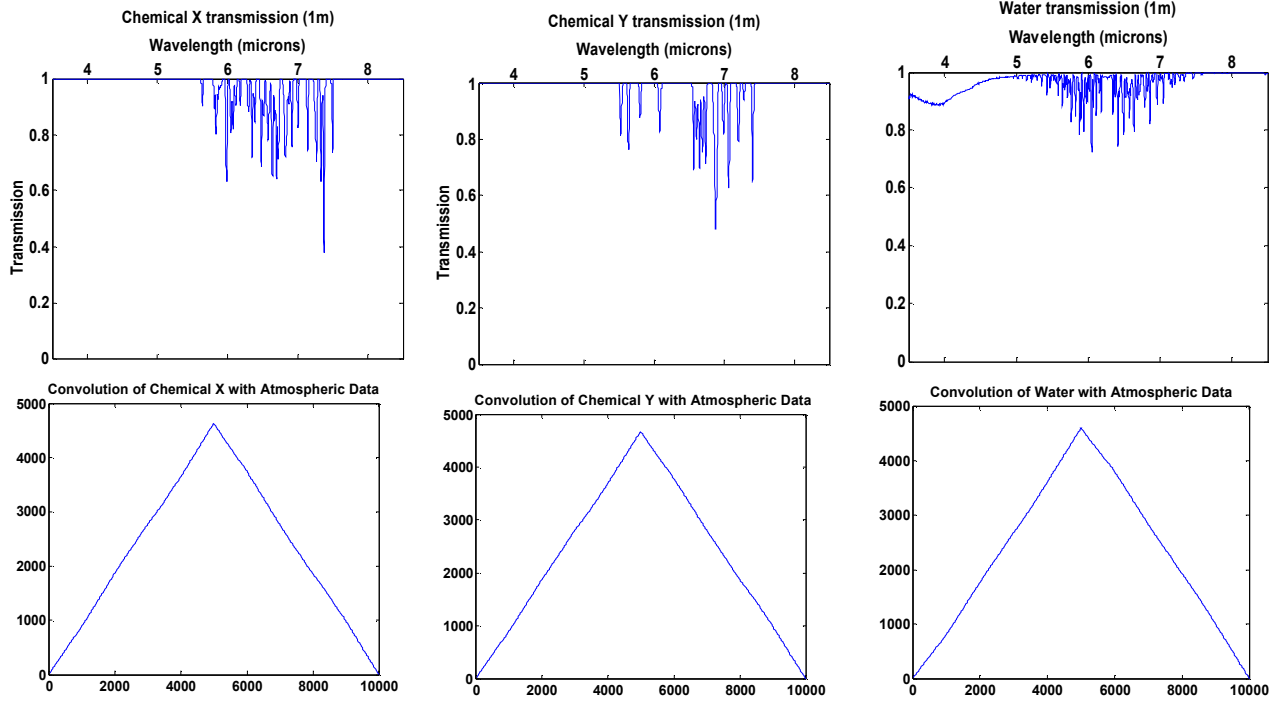


Figure 3. a. and b. are spectra representing random water-like peaks. Figure c) is a measured water spectra; all from 3.5-8.5 microns. Figures d), e), and f) are the resulting convolutions. No difference is detectable, indicating that the presence of water is not definitive.

### 3. RSG FILTER DESIGNS

We avoid the fabrication problems associated with thin film filters by using RSGs as our filter element. Now we may follow wafer-level depositions with lithographic patterning to discriminate spectral responses from one pixel to the next. The material choices available in the MWIR are limited, as many materials have absorption bands in this range. We chose ZnS and Ge as our materials for both the transmissive and reflective designs. These materials provide a low and high index of refraction for the RSG and thin film functions. Due to the long wavelengths, the grating periods are large and achievable, though etch depths and layer thickness tolerances are challenging. All simulations of the filter designs use rigorous coupled wave analysis (RCWA).

#### 3.1 Reflective Filter

The first design is an RSG in a standard reflective configuration. The reflective design as illustrated in Figure 4 is easier to fabricate than the following transmissive design. It requires only two material depositions with one shallow etch step. The same material sets may be used for both CO<sub>2</sub> and H<sub>2</sub>O monitoring filters, with the design differences shown in Table 1. Inside the CO<sub>2</sub> and H<sub>2</sub>O bands the only difference pixel-to-pixel is the lithographically defined period. From the CO<sub>2</sub> to H<sub>2</sub>O bands, the wavelength difference is too great to remain with the same material thicknesses. However, both sets of filters could be made on a single substrate if proper masking is used during deposition.

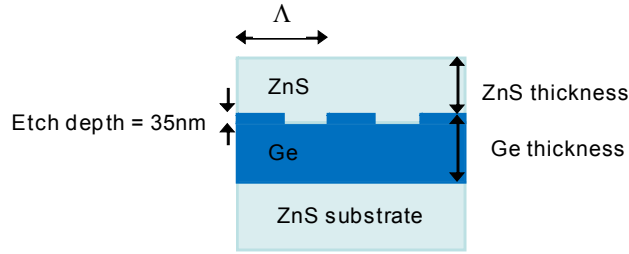


Figure 4. Reflective narrowband filter design for the midwave IR. Thicknesses are dependent on the wavelength band of interest and are given in Table 1.

<u>CO<sub>2</sub> Band</u>	<u>H<sub>2</sub>O Band</u>
4.15-4.40 $\mu$ m	5.15-5.25 $\mu$ m
Period = 1517-1633nm	Period = 1965-1994nm
Ge thickness = 450nm	Ge thickness = 500nm
ZnS overcoat = 330nm	ZnS overcoat = 430nm
35nm etch depth	35nm etch depth
50% duty cycle	50% duty cycle

Table 1. Device parameters for CO<sub>2</sub> and H<sub>2</sub>O reflective filters as depicted in Figure 4.

As an example, the reflected signal for the TM polarization is shown for 31 CO<sub>2</sub> band filters in Figure 5. While the top overcoat ZnS layer is not a requirement for RSG operation, it is necessary to reduce out-of-band reflections. By choosing the layer thicknesses judiciously, the sidebands across the measurement band can be made very close to zero. The filters have a FWHM of around 0.6nm. Periods range from 1.575 $\mu$ m to 1.725 $\mu$ m.

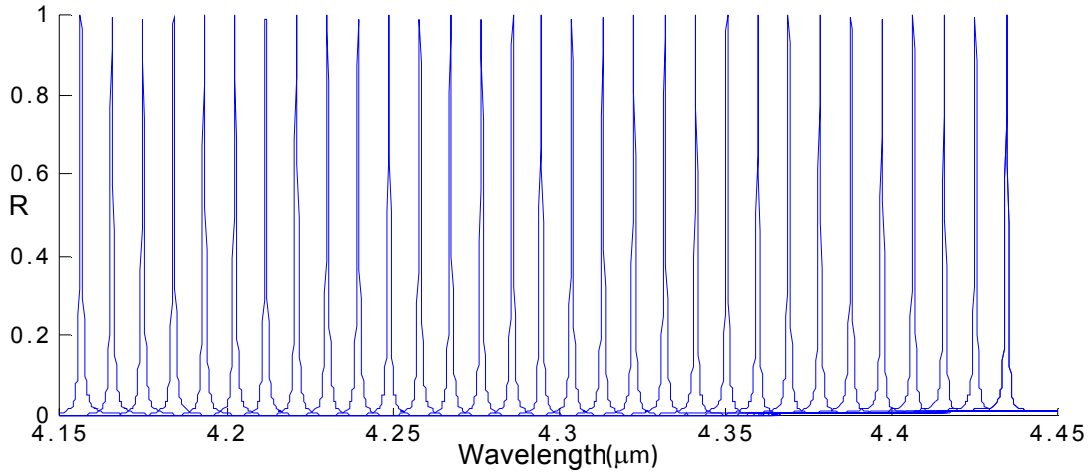


Figure 5. Reflected signal for TM polarized light from 31 gratings as simulated using rigorous coupled wave analysis. Note the extremely low sidebands of all filters. Filters differ only in grating period.

If the filters of Figure 5 were used with a pixelated detector, the light spectrum incident on an individual pixel of the FPA is the light transmitted through 1m of atmosphere multiplied by the corresponding filter response. The FPA detector element would then detect a power that is the integral of this incident spectrum over the bandwidth of the detector responsivity or the bandwidth of any other limiting filter element in the optical path. Figure 6 shows the transmitted light as a solid curve. Red squares represent the integrated signal for each filter of Figure 5. The simulated signal strength at each detector pixel tracks the shape of the absorption bands.

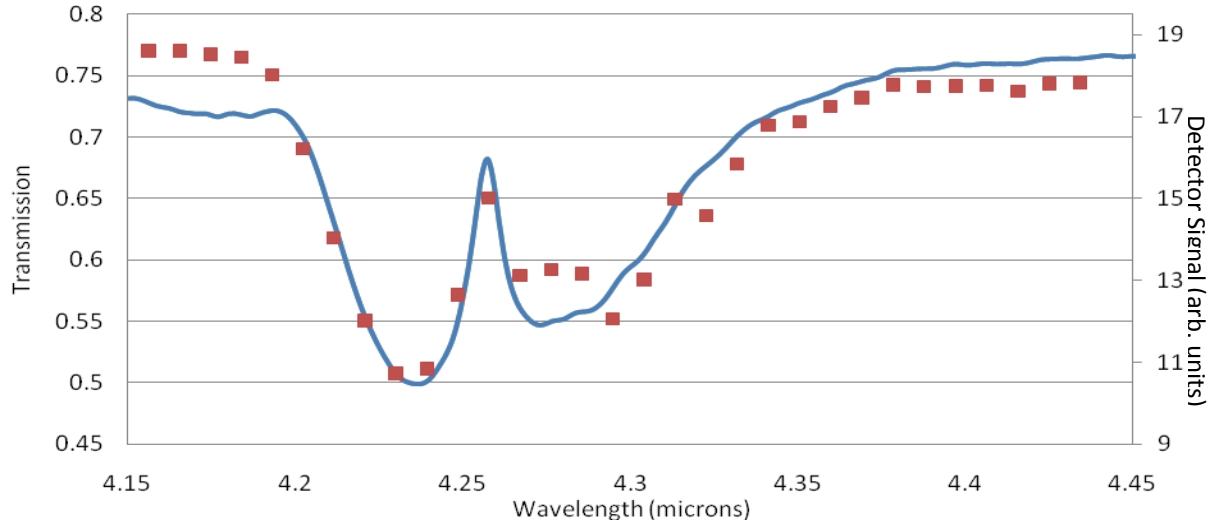


Figure 6. The solid blue curve is the measured transmission through 1m of atmosphere. The red squares represent the integrated optical power across the wavelength band for each filter of Figure 5. This value would correspond to the output signal level of a detector pixel.

#### 4. TRANSMISSIVE FILTER

In the transmissive design, the wavelength filtering function of each pixel in the optical filter array is based upon an etched Fabry-Perot micro-cavity; allowing spectral resolution with independent choice of center wavelength. The utility of this design in greatly diminishing the number of layers of material required has been previously established in [5]. Extremely narrow band filters with precise wavelength control are made possible by substituting tailored RSGs for the traditional multi-layer thin-film top mirror. The RSG can be geometrically scaled to access a wide center-wavelength range and maintain a very narrow waveband (0.1-10nm). Sandia has previously demonstrated a high-efficiency RSG [6], and a wavelength-specific pixelated filter array in the long-wave IR.[7] We combined these prior technologies to form a micro-optical component in the MWIR with a broader band Fabry-Perot cavity to realize a multitude of individual pixels in an optical filter array.

A basic design for the transmissive filter is shown in Figure 7. The lower mirror stack has a broader reflectivity peak than the narrow reflectivity peak of the RSG top mirror. As the period of the RSG is varied, the transmission peak of the entire structure varies. As in the reflective case the period is the only parameter that changes from pixel to pixel.

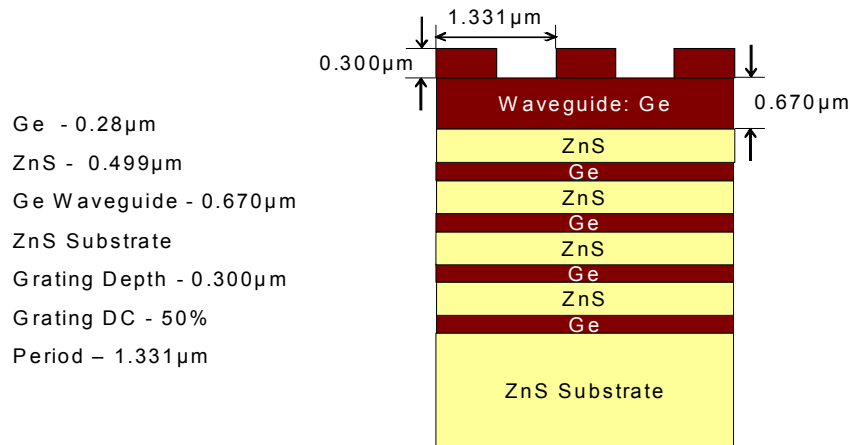


Figure 7. Transmissive narrowband filter configuration for the midwave IR illustrating top RSG element whose filter response may be varied lithographically.

In a similar manner to the reflected spectra of the filters in the prior section, the transmitted signal of these filter pixels are narrowband. In the left plot in Figure 8 we see the transmission of 14 transmissive filters, the difference in these filters is the period of the top grating period only. At right in Figure 8 we see the relationship between the period and the transmitted signal. As in the case of the reflective configuration, this relationship is near linear.

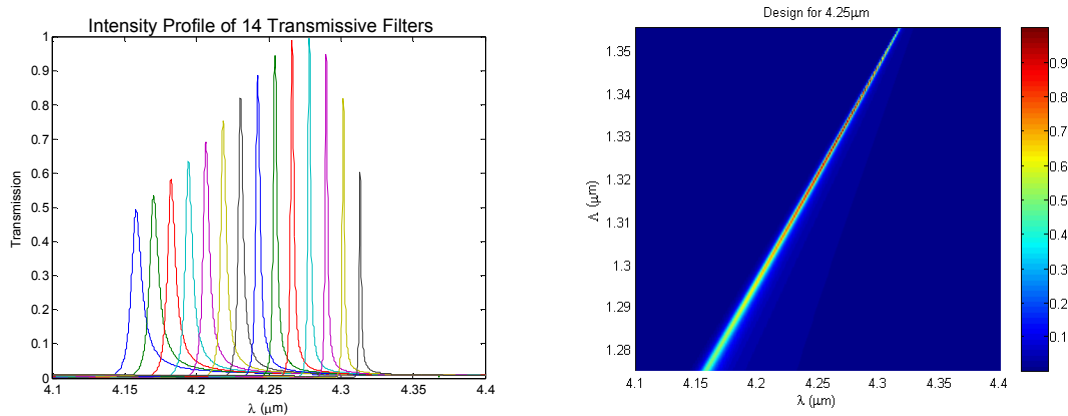


Figure 8. At left is the simulated transmission profile for 14 filters. At right is a simulation of the transmission filter for a range of periods between 1.27 to 1.36 $\mu\text{m}$ . This design provides a response in the CO<sub>2</sub> absorption band.

One drawback of this preliminary transmissive design is that the filter response varies as a function of wavelength. As can be seen in Figure 8, the transmission varies as the RSG reflection peak moves across the reflection peak of the bottom mirror. Further design optimization of the RSG and mirror stack could lead to more uniform transmission responses.

## 5. SUMMARY

We presented a reflective and transmissive narrowband filter array design in the midwave infrared (MWIR) for greenhouse gas monitoring. These filters are approximately 1nm in bandwidth, allowing us to resolve the fine features present in both the in the MWIR. The filters employ a resonant subwavelength grating (RSG) as a critical element, thus allowing lithographic definition of the filter peak wavelength. This feature enables pixelated designs on a single substrate that can cover the entire CO<sub>2</sub> or H<sub>2</sub>O absorption band. Use of ZnS and Ge ensures low absorption and high performance in the MWIR.

## 6. ACKNOWLEDGEMENT

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