Experimental Demonstration of Infrared Spectral Reconstruction using Plasmonic Metasurfaces

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We computationally reconstruct short to long-wave infrared spectra using an array of plasmonic metasurface filters. We illuminate the filter array with an unknown spectrum and measure the optical power transmitted through each filter with an infrared microscope to emulate a filter-detector array system. We then use the recursive least squares method to determine the unknown spectrum. We demonstrate our method with light from a blackbody. We also demonstrate it with spectra generated by passing the light from the blackbody through various materials. Our approach is a step towards miniaturized spectrometers spanning the short to long-wave infrared based on filter-detector arrays. © 2018 Optical Society of America

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Infrared (IR) spectroscopy is an important analytical tool for many applications, being extensively used in the pharmaceutical industry [1] and in forensic science [2] for example. The current workhorse system is the Fourier-transform infrared (FTIR) spectrometer. These offer very high resolution but are often large, heavy and expensive, and thus frequently confined to dedicated laboratory settings. IR spectrometers that are cheaper, smaller and lighter than FTIR systems might be beneficial for those in-field applications for which very high resolution is not required.

One approach for miniaturizing IR spectrometers involves the use of an array of filters rather than an interferometer (as in an FTIR system) for spectral discrimination. It has been shown that using a filter array with a detector array allows for the creation of miniaturized spectrometers [3-8]. Visible and near-infrared demonstrations have been performed with filter arrays consisting of quantum dots [3], Fabry-Perot etalons [4], multilayer photonic crystals [5], diffraction gratings [6] and microdonut resonators [7]. These types of filters often require complicated or multiple fabrication processes however, thereby increasing cost.

Recently, plasmonic metasurfaces functioning as spectral filters have been used for spectral reconstruction [8-10]. From a manufacturing standpoint they have the advantages that they can consist of a single layer of a patterned metal and that the filter function (e.g. stop band wavelength) can be modified by changing the design of nanopattern while maintaining the film thickness. Jang et al demonstrated adaptive multispectral imaging in the mid-IR using plasmonic hole arrays imaged with an IR camera [10].

In this work we demonstrate computational spectroscopy over the short-to-long-wave infrared (1.5 – 19 µm). This represents a far broader spectral range than the previous reports of Refs [3-10]. This is done using an array of plasmonic metasurfaces (Fig. 1) that act as filters for transmitted light. The computational spectroscopy is performed as follows. The filter array is illuminated with the unknown spectrum. The optical power transmitted through each filter is then measured with an FTIR microscope. The recursive least squares (RLS) method [11] is then used to determine the spectrum. This takes as its inputs the optical power transmitted through each filter and the transmission spectra of the filters.

We demonstrate our method by reconstructing five different spectra. The first is a blackbody source that consists of the globar of our FTIR system. The others are generated by passing light from the globar through the following materials: double-side polished undoped silicon (Si), single-side polished doped Si, glass and polyethylene. We show that this allows
us to determine the transmission spectra of these materials. We compare our results (reconstructed spectra) with spectra measured directly by our FTIR system and find them in reasonable agreement. We use our FTIR microscope to measure the power transmitted through each filter to emulate what would be measured by each element of a detector array matched to the filter array. The future integration of our filter array with such a detector array could form the basis for lightweight, portable and inexpensive IR spectrometers.

Each metasurface filter consists of a square array of gold blocks on a double-sided polished undoped Si substrate (float zone, $n_{ss} \approx 3.4$). The gold is 30 nm thick, with palladium (10 nm) for adhesion. Each filter has an overall extent of $\sim 100 \times 100$ $\mu$m$^2$, and is fabricated by e-beam lithography, e-beam evaporation and lift-off. The filter unit cell is shown as Fig. 2a. The filter periods vary from $P = 0.25$ to 6 $\mu$m in increments of 50 nm, i.e. 116 filters. We set the gold block length to be half the period ($L = P/2$). A scanning electron microscope (SEM) image of part of a filter is shown as Fig. 2b. Due to fabrication error, the blocks of this filter are asymmetric ($\sim 510$ nm $\times \sim 580$ nm), but this does not prevent their use for spectral reconstruction. The horizontal and vertical periods of the filters are accurately fabricated. An optical microscope image of a filter ($P = 6$ $\mu$m) is shown as Fig. 2c. Part of the filter array is shown as Fig. 2d.

The optical properties of these metasurface filters can be understood by thinking about the gold blocks as resonant antennas [12-14]. We make use of the resonance corresponding to the antenna length $L$ being half the effective wavelength in the substrate [13]. This can be rewritten in terms of the free-space incident wavelength, $\lambda_0$, that resonates with the antenna as follows:

$$\lambda_0 = 2n_{ss}L, \quad (1)$$

Where $n_{ss}$ is the substrate refractive index. At this wavelength, one would expect a dip in transmission, due to the resonant excitation of surface plasmons at the gold-silicon interface, and the accompanying increased absorption and scattering. We fabricate arrays of gold blocks (rather than isolated blocks). This modifies the resonances [15]. As we see below however, Eqn (1) still provides an excellent estimate of the resonant wavelength.

We next measure the transmission functions of the filters using an FTIR microscope system (Perkin Elmer, Frontier/Spotlight). The absolute transmission spectrum of a filter ($P = 2$ $\mu$m) is shown as Fig. 3a, obtained by measuring the transmission spectrum through the filter and normalizing by the transmission spectrum measured through an air reference path. We simulate the absolute transmission spectrum using the finite difference time domain (FDTD) method (Fig. 3a). The measured and simulated spectra are in reasonable agreement (Fig. 3a). Possible reasons for the differences that exist are discussed below. In Fig. 3b, we plot the measured transmission spectra of all 116 filters. It can be seen that Eqn (1) provides a reasonable approximation to the spectral position of the transmission dip. Fig. 3b confirms that the fabricated metasurfaces exhibit filter features (spectral dips) that can be tuned across the wavelength range of 1.5 $\sim$ 19 $\mu$m.
the FDTD method to find the transmission \( T_2 \) and reflection \( R_2 \) coefficients at the Si-air interface at which the gold block antennas are situated. The illumination is a plane wave from within the Si substrate at an angle of 10° (\( \sim \arcsin (NA/n_d) \)). We furthermore use the Fresnel coefficients to find the reflection coefficient \( R_3 \) for intensity at the Si-air interface (no antennas), with the illumination again from within the Si at 10°. The total transmission is then calculated using:

\[
T_{\text{total}} \approx T_1 T_2 (1 + R_2 R_3 + R_2^2 R_3^2 + \cdots)
\]  

(2)

The calculations are performed for both s- and p-polarizations, and the results are averaged. This method adds the intensities of the multiply-reflected waves, rather than their electric fields. This is a reasonable assumption, as the silicon wafer is very thick in comparison to the effective wavelength on resonance.

For each filter we integrate the transmitted through each filter. This represents \( R_2 \) coefficients to find the reflection coefficient at the Si-air interface at which the gold block antennas are situated. The total transmission is then calculated using:

\[
R^2 R_3
\]

The results are averaged. This method adds the intensities of the multiply-reflected waves, rather than their electric fields. This is a reasonable assumption, as the silicon wafer is very thick in comparison to the effective wavelength on resonance.

We next discuss spectral reconstruction. We begin by reconstructing the FTIR’s blackbody (globar) source. We measure the spectrum \( S_\lambda \) transmitted through each filter. This represents

\[
S_\lambda = g(\lambda) \times MCT\text{resp}(\lambda) \times T_i(\lambda) \times M(\lambda),
\]

(3)

where \( g(\lambda) \) is the globar’s spectrum, \( MCT\text{resp}(\lambda) \) is the responsivity of the mercury cadmium telluride (MCT) detector of the FTIR and \( T_i(\lambda) \) is the absolute transmission of the \( i \)th filter.

For each filter we integrate \( S_\lambda \) to give the total transmitted signal, to emulate what would be measured by a single photodetector (that is not part of an FTIR system). We term this the \( S \)-vector (1×116, Fig. 4a). We form filter matrix \( T \) from the transmission spectra \( T_i(\lambda) \) of the filters.

Each spectrum contains data for 116 wavelengths, so \( T \) is a square matrix (116×116, Fig. 3b), \( S \) and \( T \) are the inputs to the RLS method that then reconstructs the (previously unknown) spectrum: \( R(\lambda) = g(\lambda) \times MCT\text{resp}(\lambda) \). We first apply this approach to reconstruct the globar source of our FTIR system. The reconstructed spectrum is in good agreement with the spectrum measured directly by the FTIR (Fig. 4b). We further quantify this by the normalized mean-absolute-error (NMAE). The NMAE is the mean of the absolute differences between the measured (by FTIR) and reconstructed spectra, normalized to the peak signal value. The reconstructed globar spectrum has NMAE=0.025.

We next repeat this technique to reconstruct spectra generated by passing light from the globar through various materials. The material to be tested is placed between the FTIR spectrometer (Perkin Elmer, Frontier) and microscope (Perkin Elmer, Spotlight). The measured spectrum transmitted through each filter is now:

\[
S^M_\lambda = g(\lambda) \times MCT\text{resp}(\lambda) \times T_i(\lambda) \times M(\lambda).
\]

(4)

where \( M(\lambda) \) is the transmission spectrum of the material. The reconstructions are carried out using the filter matrix \( T \) measured previously. The RLS method is again applied, this time reconstructing the following quantity:

\[
R^M(\lambda) = g(\lambda) \times MCT\text{resp}(\lambda) \times M(\lambda)
\]

(5)

We then use this and the reconstructed globar spectrum to find the transmission spectrum each material as follows:

\[
M(\lambda) = R^M(\lambda)/R(\lambda)
\]

(6)

The results are shown as Fig. 5a-d. The reconstructions are in reasonable agreement with the transmission spectra measured directly by the FTIR system (by placing the sample on the FTIR microscope). This is evidenced by the relatively low NMAE value for each reconstruction. The largest deviations between the reconstructed and directly measured spectra of Fig. 5a-d occur at the edges of the spectral range, i.e. for \( \lambda < 2 \mu m \) and \( \lambda > 16 \mu m \). Indeed, the reconstructed material transmission spectra for Fig. 5a-c take negative values near \( \lambda = 1.5 \mu m \), which is clearly unphysical. Similarly, the reconstructed spectra of Fig. 5c & d exceed unity at short and long wavelengths, respectively, which is again unphysical. A possible reason for the greater inaccuracies at the edges of the reconstruction spectral range is that the globar source provides smaller signal there. In addition, one might expect the reconstruction performance to be compromised for wavelengths that are closer to the edges of the reconstruction spectral range than the spectral width of the stop band of each plasmonic filter. Future work on filters with narrower spectral features could be a means to mitigate this issue.

![Fig. 4.](image-url)

(a) Integrated transmitted signal of each filter (S-vector). (b) Reconstruction of globar source (NMAE = 0.025).
Fig. 5. Reconstructed transmission spectra of (a) double-side polished undoped Si (NMAE = 0.066), (b) single-side polished p-doped Si (1-100 ohm cm, NMAE = 0.091), (c) glass (NMAE = 0.094) and (d) polyethylene (NMAE = 0.089). (e) Normalized error (red, left axis) and globar signal (blue, right axis) vs wavelength.

It can be seen from Fig. 5d that the reconstructed polyethylene spectrum shows dip features around the appropriate wavelengths, but that these are far wider than those of the spectrum directly measured by the FTIR. This is likely due to the transmission dips of the spectrum being far narrower than the transmission features of the filters. Using band-pass filters with higher resolution features [17, 18] could allow for the accurate reconstruction of sharp features like those of polyethylene and other plastics.

In conclusion, we demonstrated proof-of-concept for short- to long-wave IR spectroscopy with an array of plasmonic metasurface filters. We anticipate that future works on plasmonic metasurfaces with narrower spectral features and integration with detector arrays could be fruitful.

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References and links
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