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# Material identification by plasmonic infrared microspectrometer employing machine learning

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**Abstract:** We demonstrate a microspectrometer comprising plasmonic filters integrated with an infrared camera. Blackbody light illuminates the material being studied, with transmitted light collected by the microspectrometer. The latter uses machine learning to identify the material.

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## 1. Introduction

Mid-infrared (MIR) spectroscopy enables materials to be identified and quantified. It therefore has a wide range of applications, including biosensing, hazardous chemical detection and environmental monitoring. The current workhorse tool for MIR spectroscopy is the Fourier transform infrared (FTIR) spectrometer. This has high resolution and is suitable for many applications. However, there are many scenarios for which the size, weight and budget for the tool are limited and for which only modest resolution is needed. This motivates the development of compact and cost-effective MIR microspectrometers [1, 2].

Here we demonstrate a filter array-detector array (FADA) microspectrometer consisting of a plasmonic mid-infrared (MIR) spectral filter array integrated with a thermal infrared camera (FLIR Lepton). We post-process the raw image outputs from the camera to train a machine learning (ML) classification model to identify samples. These include semiconductor substrates (undoped silicon, GaAs, glass and quartz). In addition, photoresist films (AZ series from MicroChemicals), e-beam resist films (MicroChem 950PMMA A series) and epoxy resin (MicroChem SU-8 3000 series) films on undoped silicon substrates are studied. We demonstrate that the ML model can identify samples with high accuracy.

## 2. Device Design

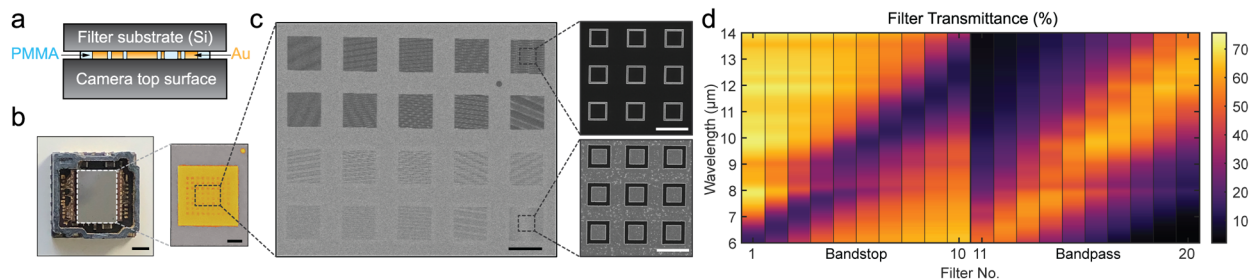


Figure 1: (a) Device schematic. (b) Photo of bonded device (left, scale bar: 2 mm) and plasmonic filter chip (right, scalebar: 1 mm). Weight of camera module after filter bonding is 1.1 g. (c) Left: SEM images of fabricated plasmonic filter array (scalebar: 100  $\mu\text{m}$ ). Right: SEM images of bandstop (top) and bandpass (bottom) filters (scalebars: 3  $\mu\text{m}$ ). (d) Measured filter transmittance spectra.

Fig. 1a shows the schematic of the device, comprising a plasmonic filter array on an undoped silicon substrate (500  $\mu\text{m}$  thick) bonded on to a thermal camera using PMMA resist. The spectral response of the camera (FLIR Lepton) covers the mid-IR wavelength range from 6 to 14  $\mu\text{m}$ . The filter array contains twenty filters, with each having an extent of  $100 \times 100 \mu\text{m}^2$ . The filter chip is fabricated by e-beam lithography, e-beam evaporation of gold (150 nm thick) and the lift-off process. The completed microspectrometer (i.e. after filter bonding) is shown as Fig. 1b. The twenty filters are divided into two categories: bandstop filters (square arrays of rectangular gold rings) and bandpass filters (square arrays of rectangular coaxial apertures on gold). We have previously used related structures for computational IR spectroscopy [3, 4]. SEM images of the filters are shown as Fig. 1c. The geometric parameters, e.g. ring outer length, ring width, gold thickness and array period, determine the resonances supported by the plasmonic structures. Transmittance spectra of the filters measured by FTIR are presented as Fig. 1d. For the bandstop and bandpass filters, the array period  $P$  varies 1.8 to 3.6  $\mu\text{m}$  and from 1.9 to 3.7  $\mu\text{m}$ , respectively (both in steps of 200 nm). It can be seen that the bandstop and bandpass features both shift to longer wavelengths with the period.

### 3. Result and Discussion

Transmission spectra of the samples used for testing are shown as Fig 2a. Fig.2b shows the experiment setup where a blackbody calibrator (OMEGA BB703 set at 573.15 K) is used as the mid-IR source. The sample to be tested is placed directly in front of the flat-field-correction (FFC) shutter of the Lepton module. In Fig. 2c we show a typical raw (i.e. unprocessed) sensor output. The top/bottom two rows are the bandstop/bandpass channels.

The raw output (corresponding to each filter) can be considered to be the product of the IR source spectrum, sample transmittance spectrum, filter transmittance spectrum and detector responsivity spectrum, integrated over wavelength. We perform the following to get the readout value of each filter channel. We begin by averaging the pixel readout values of the selected area (white dashed lines in Fig. 2c) for each filter channel. These are then normalized by data collected with no sample in place. The processed data is shown as Fig. 2d, with error bars given by the standard deviation found from 150 measurements made on each sample. The data for the ten bandstop channels are plotted with darker color than the data for the ten bandpass channels (see caption Fig. 1d). It can be seen that the samples show highly distinctive readout values. The glass, quartz and GaAs samples have noisier readout values than the resist samples due to their significantly lower transmittance, which leads to smaller signals at the detector end.

We further perform principal component (PC) analysis on the data. Its visualization in the space of the first two PCs is shown as Fig. 2e. Each sample class forms a closely-packed cluster, which is advantageous for ML training. We train a support vector machine (SVM) classification model. The five-fold cross-validation result is 100 % for all samples, based on 150 measurements per sample. We next plan to use this for liquid and gas chemical identification.

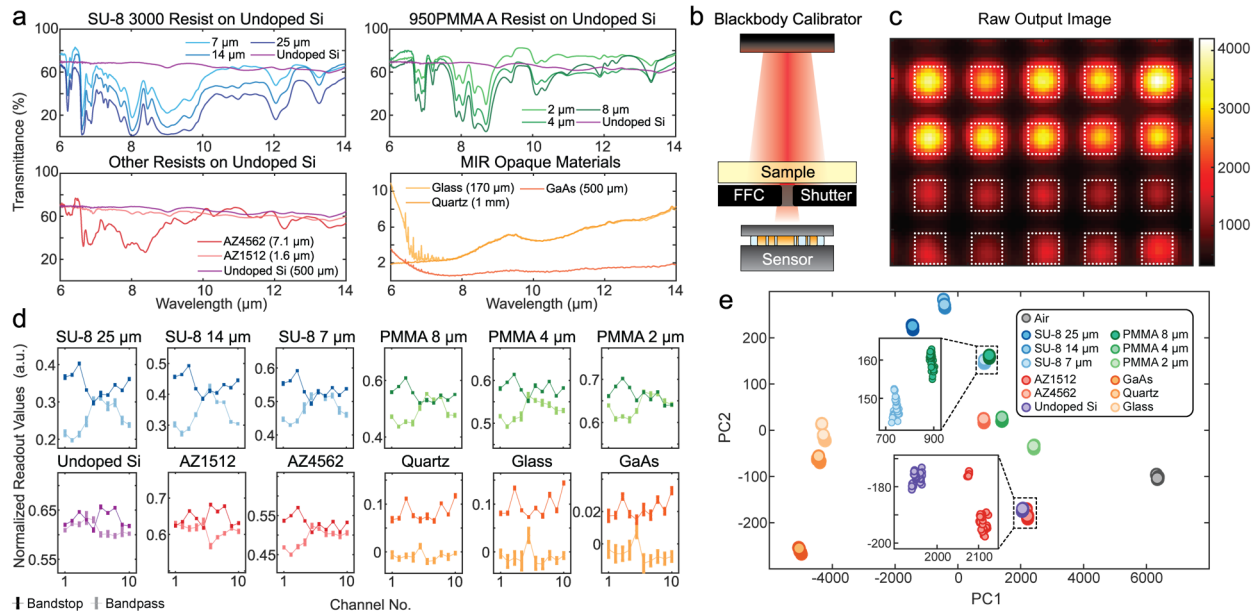


Figure 2: (a) Transmittance spectra of different materials. (b) Experimental setup. (c) Raw output image of undoped Si with the color scale indicating readout values (a.u.). (d) All readout data after postprocessing. (e) Principal component (PC) analysis of the training data.

### 4. Acknowledgement

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