

Planar integrated plasmonic mid-IR spectrometer

P. Figueiredo^a, J. Nath^a, G. Medhi^a, A. Muraviev^a, C. J. Fredricksen^b, W. R. Buchwald^c,
J. W. Cleary^d, R. E. Peale^{a,*}

^aDept. of Physics, Univ. of Central FL, 4000 Central Florida Blvd. Orlando, FL 32816

^bLRC Engineering, 9345 Chandon Drive, Orlando, FL USA 32825

^cSolid State Scientific Corporation, 27-2 Wright Road, Hollis, NH 03049

^dAir Force Research Laboratory, Sensors Directorate, 80 Scott Dr., Hanscom Air Force Base, MA
01731

*Robert.Peale@ucf.edu

ABSTRACT

Mid-IR spectrometers with adequate resolution for chemical sensing and identification are typically large, heavy, and require sophisticated non-stationary optical components. Such spectrometers are limited to laboratory settings. We propose an alternative based on semiconductor micro-fabrication techniques. The device consists of several enabling parts: a compact broad-band IR source, photonic waveguides, a photon-to-surface-plasmon transformer, a surface-plasmon sample-interaction region, and an array of silicon ring-resonators and detectors to analyze the spectrum. Design considerations and lessons learned from initial experiments are presented.

Keywords: Compact FTIR Spectrometer, surface plasmon polariton, micro-ring resonators

1. INTRODUCTION

We propose a compact mid-IR spectrometer based on a broad-band light source, dielectric waveguides, a transformer to convert between waveguide modes and surface plasmon polaritons (SPP), an interaction region where analyte molecules are interrogated by SPPs, an array of ring resonators to disperse the light into spectral components, and photodetectors. A light source will emit into a dielectric waveguide, which will lead to a region which will allow coupling of the incident photons into SPPs. These will propagate along a functionalized metal surface within a sample interaction zone. This functionalized metal surface will allow interactions between the propagating SPP and any analytes bound to the surface, causing increased loss at those wavelengths that correspond to the analyte vibrational modes. After a suitable propagation length the SPP will be coupled back into a dielectric waveguide, where specific wavelength components will be out-coupled to detectors by an array of ring resonators. The simplest useful spectral sensor of this design would have two spectral channels. The use of SPPs in the interaction region favors application to surface bound molecular analytes, such as biomolecules bound to antibodies attached to the functionalized conductor surface.

To illustrate the concept, Fig. 1 presents a schematic of one particular vision for the device. Here, the broad-band source of mid-IR radiation is a multimode quantum cascade laser. The photonic waveguide is a silicon ribbon bonded to a ZnO substrate, a medium with index lower than silicon's and having low mid-IR loss. The taper is formed photolithographically and is separated from a recessed gold film by a distance comparable to the wavelength, so that evanescent fields from the silicon may excite SPPs on the gold. The SPPs propagate along the gold, with their spectrum selectively altered via absorption by analyte molecules, until they reach a second taper that couples the SPPs back into a photonic waveguide. A single ring-resonator is shown for outcoupling one of the spectral components of the radiation to a detector. The details in the Fig. 1 design concept are for illustration only, and initial investigation of each subcomponent has already led to significant changes, as discussed next.

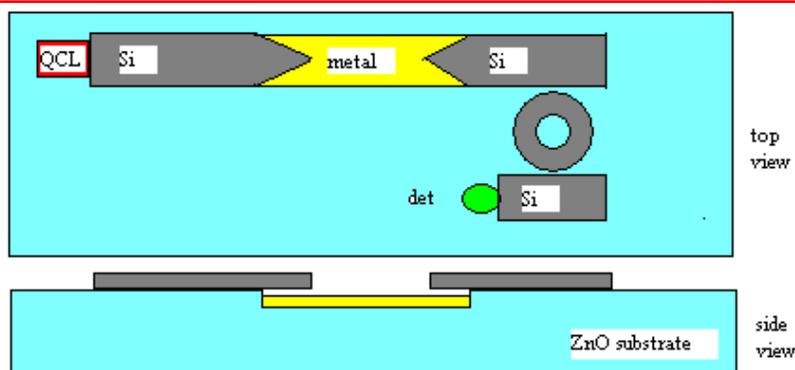


Figure 1. Schematic device, consisting of QCL source, Si waveguide on a ZnO substrate, photon/SPP transformer, depressed metal-coated sample-interaction region, SPP/photon transformer, Si outcoupling waveguide, micro-ring resonator, and detector.

2. MID-INFRARED BROAD-BAND SOURCE

The initial device concept (Fig. 1) imagined a multimode quantum cascade laser (QCL) as the broad band IR source. Our experiments on commercial QCLs showed that the spectrum may be as broad as 60 cm^{-1} with a $\sim 1 \text{ cm}^{-1}$ mode spacing when operated in pulsed mode with a pulse duration of $\sim 100 \text{ ns}$ and a duty cycle of a few percent (Fig. 2, left). However, when the pulse duration is extended to ms and longer, mode competition causes the laser to operate over a much more restricted wavelength range of just a few wavenumbers, which is much less than usual molecular bandwidths (Fig. 2, right). This spectrum is very sensitive to temperature and operating conditions, and it changes during the pulse as the active crystal is heated by the excitation current. Moreover, the cost of QCL chips is still very high, of order \$5000, not counting any support equipment such as temperature controlled housing or laser driver. An additional consideration is that QCLs are unavailable presently at wavelengths as short as 2.8 microns, where important characteristic molecular vibrations occur based on stretches in the bonds of C-H (Alkynes), O-H (monomeric alcohols, phenols) and N-H (Amines). For these reasons we consider QCLs unattractive as the source of IR broad-band radiation in the considered device.

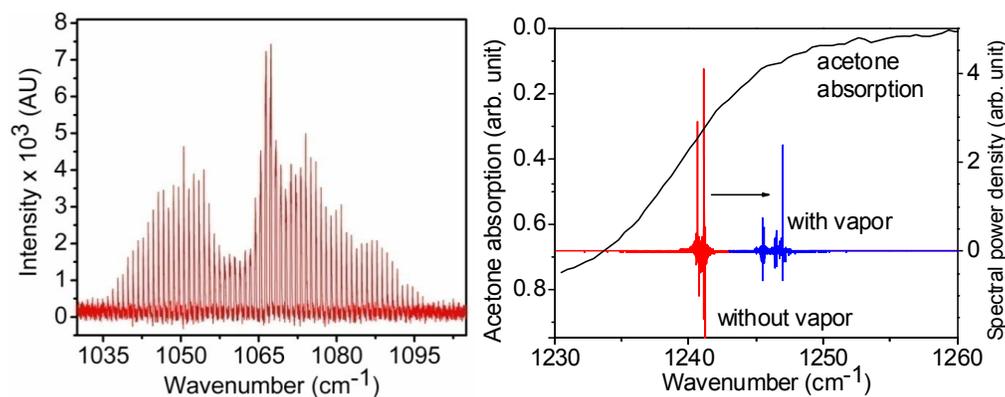


Figure 2. Comparison of pulsed and cw QCL spectra. (left) ALPES 9.3 micron QCL operated with 100 ns pulses showing 60 cm^{-1} emission bandwidth. (right) Continuous wave Maxion 8.1 micron QCL spectrum together with the absorption spectrum of acetone. The shift in the laser spectrum caused by intracavity acetone absorption¹ is evidence that the QCL gain bandwidth is much larger than the emission bandwidth. Both lasers have comparable gain band width, but the emission bandwidth of the cw laser is only a few wavenumbers, much less than the absorption bandwidth of typical molecules.

We turn our attention next to mid-IR LEDs. A suite of these were purchased from Boston Electronics at a cost of only $\sim \$100$ each. Their spectra (Fig. 3) and temperature dependence were characterized using a Fourier transform infrared (FTIR) spectrometer (Bomem DA8, KBr beam splitter, 77 K InSb detector.) The LEDs were mounted at the spectrometer emission port. Each LED was operated at the specified maximum power conditions in continuous wave

mode, with an excitation current of 100-200 mA. Each observed band matches the center wavelength specified. Shifts with temperature, measured by attaching the LED to a thermoelectric heater/cooler, were less than the emission bandwidths. Unlike the QCL, there is no mode structure. The small feature at 4.2 micron wavelength, due to carbon dioxide absorption, already suggests their potential for molecular sensing. In comparison to QCLs, the range of available wavelengths is shifted to the blue, such that the important region of characteristic vibrations below 3 microns is accessible. Thus, IR LEDs appear to be a viable broad-band IR source for the subject device.

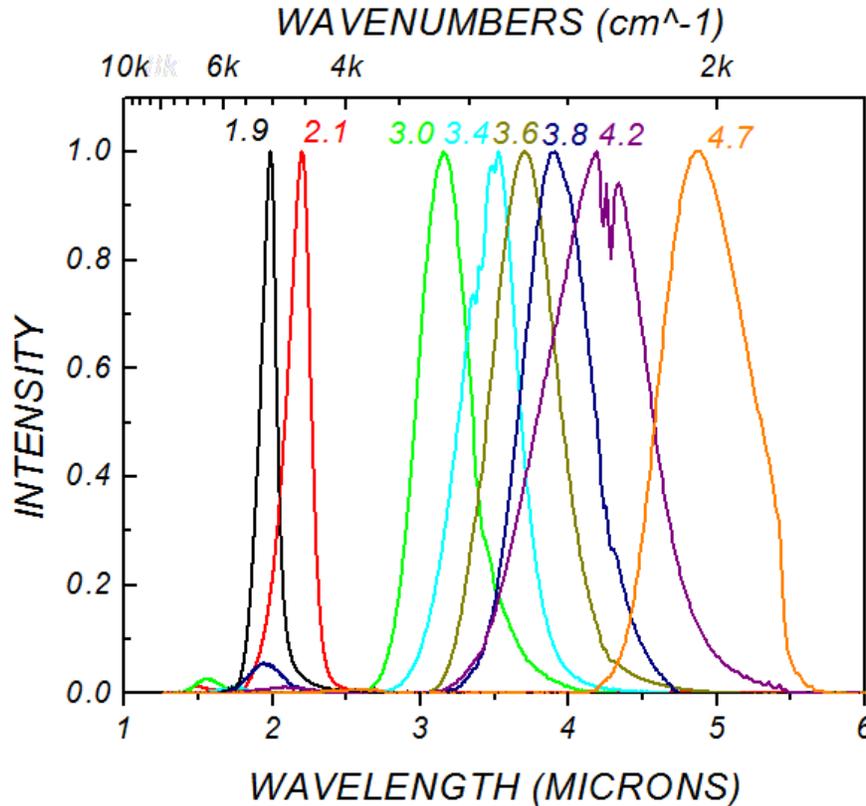


Figure 3. Infrared LED spectra. Intensity has been normalized.

3. PHOTON TO SPP COUPLER

The next objective is to demonstrate a viable conversion of waveguide photons to SPPs on a metal surface. The direct excitation of surface plasmon modes from dielectric waveguides has precedent^{2,3}. In these previous works evanescent fields originating from the dielectric waveguide appear across a low index gap and are used to provide the momentum matching condition required for efficient plasmon generation. This approach is reminiscent of the so-called “Otto configuration” of SPP generation⁴. In Ref. [2], a taper was needed to get the effective index of the waveguide to be less than the effective index of the SPP mode so that they have large evanescent fields. In Ref. [3] SPPs are simply excited across a gap. The taper appears to improve the conversion efficiency.

Although this “Otto” approach has been shown to be feasible, we favor tapered metal-clad waveguide as shown in Figure 4. In this approach, the electromagnetic wave is incident upon a section of metal-cladded waveguide tapered to a dimension such that the effective index of the waveguide will be less than the effective index of an SPP mode propagating on the surface of the metal. This method is reminiscent of the so-called “Kretschmann configuration” of SPP generation⁵ and requires the metal cladding to be thin enough such that evanescent fields can penetrate through the metal to excite SPP modes on the surface.

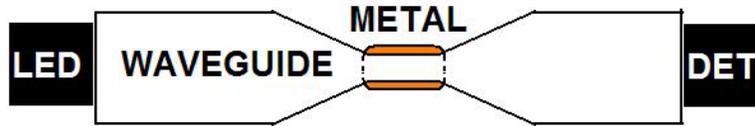


Figure 4. Schematic of metal-coated necked fiber for coupling photons to SPPs.

To gain initial insights on a photon-SPP transformer, we will first experiment with IR fiber. The IR glass chosen for our initial investigations is Gallium Lanthanum Sulphide Oxide (GLSO), which was obtained from ChG Southampton. Compared with other IR glasses, it has relatively low toxicity. It has low attenuation within the mid-IR range (Fig. 5)⁶⁻⁸. It has a refractive index of 2.37 at 1.7 micron wavelength⁶. Bulk GLSO rods will be zone heated above the solid/liquid transition temperature (580 C) to the softening point (600 C)⁶. GLS is typically drawn just below the onset of crystallization at ~700 C^{7,8}. Once the fiber is drawn to ~50 micron diameter, it will then be necessary to neck down the interaction region to a diameter of ~2 micron and a length of up to several mm. (We have observed SPP propagation on gold of ~1 cm at 10 micron wavelength^{9,10}.) Multiple drawings risk crystallization, which results in higher absorption loss, though methods are known for avoiding this^{7,8}.

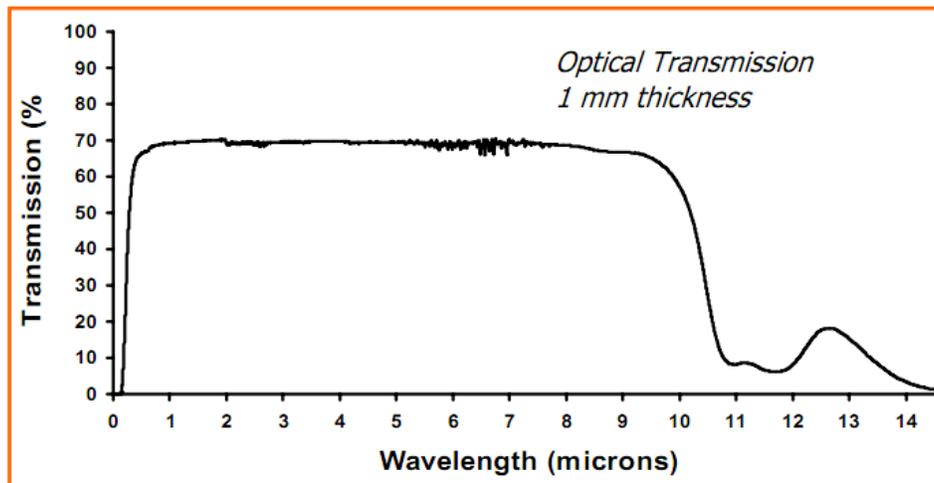


Figure 5. Transmission spectrum for GLS.⁴

A consideration for the interaction region is the metal used to support SPPs. Gold is traditional at visible wavelengths, just below its plasma frequency, where SPP mode confinement is sub-wavelength. However, the mode-confinement rapidly worsens with increasing wavelength. This reduces the overlap of the SPP field with analyte molecules bound to the surface, leading to weaker absorption signals. To obtain the highest sensitivity at mid-IR wavelengths, therefore, it is necessary to select a material with an infrared plasma frequency. Some possibilities that we have considered recently include metal silicides^{10,11}, semi-metals (Sb, Bi, graphite)¹², heavily-doped semiconductors¹⁰⁻¹³, and conducting polymer¹³.

4. RING RESONATOR

The next enabling technology is the ring resonator. Its circumference must equal an integer (m) number of wavelengths λ/n , where n is the index of refraction and λ is the vacuum wavelength. For hypothetical photons of 3.4 micron wavelength traveling through silicon ($n = 3.4$), the circumference must therefore be m microns. The free spectral range (FSR) is required to be sufficient so that opposite ends of the LED spectrum are not simultaneously resonant in one ring. At 3.4 micron wavelength a free spectral range of ~0.7 micron is needed, according to the LED bandwidths evident in Fig. 3. Since $FSR = \lambda/m$, we arrive at a required resonance order of not more than $m = 5$. According to these estimations, the ring circumference should be 5 microns.

The transverse dimensions of the ring should be comparable to the wavelength, which in silicon (for 3.4 micron vacuum wavelength) would be ~ 1 micron. Otherwise, the losses will be enormous. Together with the circumference limit defined by the FSR requirement, this leads to an unusual ring geometry, in which the ring radius and ring width are nearly the same.

The resolving power (Q) of the micro-ring resonator is dependent on its width, as a large width can allow transverse modes. We desire a $Q = \lambda/\Delta\lambda$ of at least 1000 to ensure that each ring will act as single resolution channel with a reasonably useful resolution of $\Delta\lambda = 3$ nm. This value of Q seems readily obtainable with present fabrication techniques^{14,15}. The precise requirements of the micro-ring resonator's circumference and width may be achieved in principle by photolithography. The device may be conveniently fabricated from silicon-on-insulator (SOI), where the waveguides and rings are supported by a layer of SiO_2 , which has lower index than silicon.

Unfortunately, SiO_2 is lossy in the mid-IR, and the evanescent part of the guided wave extends into it. An alternative substrate for the rings and waveguides is zinc oxide, which has low loss at 3.4 micron and its refractive index¹⁶ is 2.02, sufficiently less than silicon's for good confinement. A method known as epi-layer transfer may be used to apply thin silicon layers to the zinc oxide substrate. This is the motivation for the ZnO substrate suggested in Fig. 1.

Molecular sensing requires a minimum of two ring resonators. Such a simple spectrometer that senses just two wavelengths can function in a differential absorption mode, where one of the wavelengths coincides with a particular molecular absorption band and the other is chosen where no molecular absorption is expected. This configuration is indicated schematically in Fig. 6.

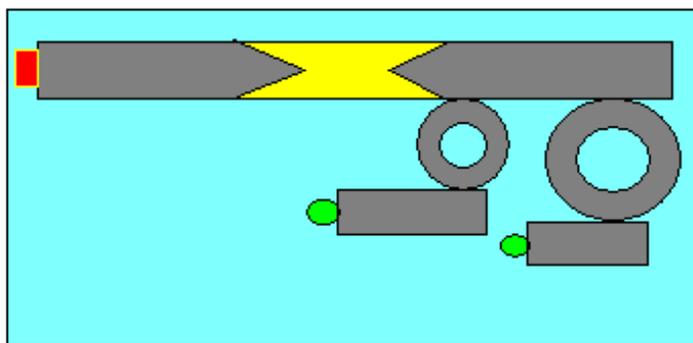


Figure 6. Schematic of two channel spectrometer.

5. SUMMARY

Design considerations for a planar integrated IR spectrometer have been presented. Enabling technologies have been identified, and preliminary investigations of feasibility presented. A relatively simple, integrated mid-IR spectrometer is proposed based on the conversion of dielectric waveguide modes to surface plasmon modes with inexpensive IR LEDs proposed as the light source. Interactions between the SPP modes and any surface bound analyte will cause characteristic absorption peaks to appear in the waveguided optical field. The resulting spectrum can be analyzed through the use of integrated narrow-band detectors formed from micro-ring resonators. The overall resolving power of this device can be increased with the addition of more micro-rings with additional sensitivity provided by the possibility of operating in a differential absorption mode. It is believed such a device will have use in portable chem/bio identification scenarios.

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