Molecular fingerprint sensing using Ge-on-Si waveguides

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***Abstract*— Germanium-on-silicon, mid-infrared waveguides are used to demonstrate molecular fingerprint sensing of poly(methyl methacrylate) between 7.5 and 10 µm wavelength. The results are compared to Fourier transform infrared spectroscopy measurements, highlighting the potential of the platform for the identification of analytes.**

Keywords—Germanium; mid-infrared; waveguides; sensing; molecular fingerprint.

I. INTRODUCTION

In recent years there has been a drive from the photonics community to develop miniaturized optical sensing systems operating at mid-infrared (MIR) wavelengths [1]. In particular, operation at wavelengths in the molecular fingerprint regime (6.7 – 20 µm) would allow for label free sensing of a number of molecules by their unique absorption spectra [2], which are key to a number of vital applications such as pollution monitoring, health care (using breath bio-markers or blood analysis) and explosive detection. New material platforms are required to establish such a system, as silicon-on-insulator technologies become lossy due to material absorption above ~3.6 µm wavelength [3]. Ge is transparent up to ~15 µm wavelength, and is of significant interest in part due to its compatibility with Si growth and foundry processes. As a result a number of groups have investigated Ge-on-Si [4,5] and Ge rich SiGe [6] platforms for integrated MIR photonic components. Previously, we have demonstrated record low losses with Ge-on-Si rib waveguides operating up to 11 µm wavelength [7]. Here, we demonstrate the potential for optical sensing applications by using Ge waveguides to evanescently sense absorption lines in poly(methyl methacrylate) (PMMA) polymer films, using a differential measurement of waveguides with and without the analyte present. It is believed that these results constitute the first demonstration of Group IV waveguide sensing in the molecular fingerprint regime. The results are compared Fourier transform infrared (FTIR) measurements; the gold standard for optical identification.

II. DESIGN AND FABRICATION

Ge epitaxial layers of 2 µm thickness were grown on (100) Si wafers by reduced pressure chemical vapor deposition. Cyclic annealing was used to reduce the threading dislocation density down to < $1x10^7 cm^{-2}$ at the top plane. The material was found to have a low background doping of < $1x10^{15}$ cm^{-3} by secondary ion mass spectroscopy, which ensures that free carrier absorption losses are negligible. The rib-waveguides are patterned using electron beam lithography and dry etched to a depth of 1 µm with a SF_6 and C_4F_8 chemistry [8]. Waveguide losses are measured by the Fabry-Perot technique using a quantum cascade laser (QCL) package that emits from 7.5 to 11.5 µm wavelength [7].

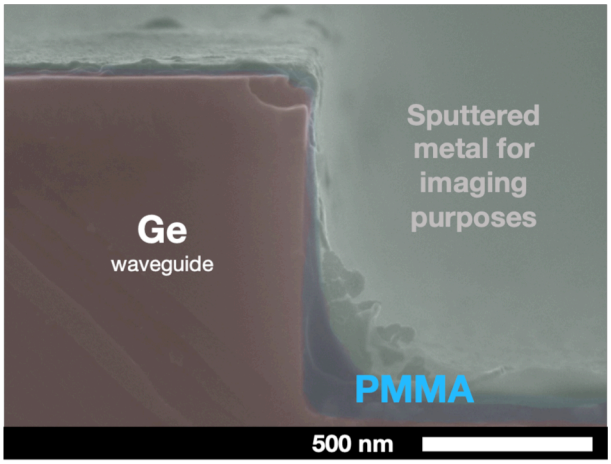

Fig. 1: A scanning electron microscope cross section of the 2 µm thick Ge-on-Si rib waveguide sidewall coated with PMMA. False coloring has been added for clarity.

As the MIR QCL laser source does not allow for continuous tuning without mode hopping, the sample index is instead tuned using a resistive heater (thermo-optic effect), in order to observe Fabry Perot fringes. We have achieved low (< 4 dB/cm) propagation losses across the measurement range in transverse electric (TE) polarization, reaching as low as ~ 1 dB/cm at ~ 10 µm wavelength [7]. A local maximum of ~ 4 dB/cm is found at ~ 9 µm wavelength. This absorption is due to an interstitial oxygen bond in the Si substrate, with which the optical mode overlaps.

III. RESULTS

In order to demonstrate optical sensing in this spectral region, the sample was spin coated with a PMMA polymer,

Fig. 1, and selectively patterned by oxygen plasma ashing to leave only a ~ 1 mm strip (i.e. a waveguide segment of ~ 1 mm length with PMMA remaining). Transmission measurements were carried out on waveguides with and without PMMA coatings, by stepping the QCL MIR source wavelength in 10 nm increments and recording the spectrum on a liquid nitrogen cooled mercury cadmium telluride (MCT) detector. Similarly, surface normal transmission measurements were taken on Si wafers with and without PMMA coatings, using a Bruker 66 V FTIR spectrometer. Dividing the spectra recovers the transmission of the PMMA spectra, shown in Fig. 2, for both FTIR and waveguide measurements.

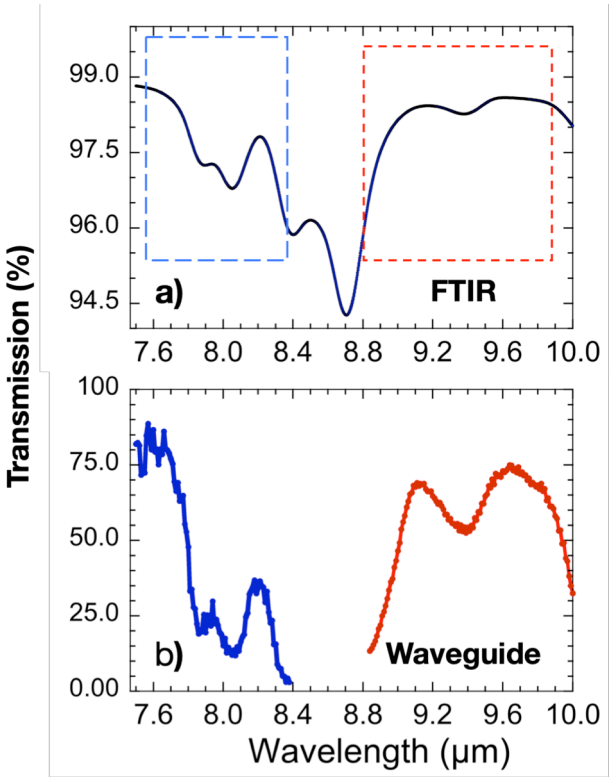

Fig. 2: Transmission measurements of poly(methyl methacrylate) films using a) Fourier transform infrared spectrometry and b) evanescent sensing using Ge–on-Si rib waveguides.

Clearly, spectral features can be observed, with absorption between ~ 8 and 9.4 μm corresponding to a range of C-O-C stretching modes in the polymer film [9]. Comparing the waveguide spectra to the transmission by surface normal FTIR, there is an enhancement factor (i.e. increased attenuation) in the waveguides due to the larger interaction length with the analyte, despite the low modal overlap in the waveguide geometry. These results demonstrate approximately a 40 times enhancement compared to surface normal FTIR (i.e. the transmission is equivalent to a surface normal measurement with a film 40 times thicker). This enhancement factor can be hugely increased by coating a larger section of the waveguide. The upper limit of this is set by the waveguide loss, as the optimum sensing length in cm is approximately ~ $1/\alpha$ [10], where α is the propagation loss in cm^{-1}. For example, with 1 dB/cm loss at ~10 μm wavelength [7] the optimum waveguide length would be 4.34 cm. For broadband measurements, with an analyte containing molecular vibrations of varying strength, the dynamic range of the measurement could be improved by using a number of waveguides, each with a sensing window of different length. Future work will focus on determining the optimum waveguide geometry for sensing based on the optical overlap and propagation loss of various waveguide dimensions.

IV. CONCLUSIONS

Molecular sensing of PMMA polymer films has been achieved using the evanescent field of Ge-on-Si waveguides, between 7.5 and 10 μm wavelength, where a number of absorption wavelengths have significantly stronger absorption than at shorter wavelengths and can be used to uniquely identify an analyte from its absorption fingerprint. Using a differential measurement, the spectral vibrations due to a range of C-O-C bonds are clearly observed, and are compared to surface normal transmission measurements taken by FTIR. An enhancement factor of ~ 40 is observed compared to surface normal FTIR. An advantage of this sensing geometry is that with low propagation losses, longer waveguides can be used to increase the interaction length with the analyte, improving the minimum concentration detectable for a given source power and detector. For certain applications, such as label free study of proteins or DNA this could hold significant advantages, where single pass surface normal measurements are not easily achievable.

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