Ge-on-Si mid-infrared waveguide platform for molecular fingerprint sensing

Kevin Gallacher[1], Ross W. Millar[1], Ugne Griskeviciute[1], Martin Sinclair[1], Marc Sorel[1], Leonetta Baldassarre[2], Michele Ortolani[2], Richard Soref[3], and Douglas J. Paul[1]

[1]*University of Glasgow, James Watt School of Engineering, Rankine Building, Glasgow, G12 8LT, UK*
[2]*Dipartimento di Fisica, Universita di Roma La Sapienza, Piazzale Aldo Moro 5, I-00185 Roma.*
[3]*Engineering Program, University of Massachusetts at Boston, Boston, Massachusetts 02125, U.S.A.*

ABSTRACT

The mid-infrared spectral region is key to several large market applications such as security, healthcare and environmental monitoring. This is due to how chemical compounds can be detected from unique vibrational modes that absorb in the molecular ‘fingerprint’ region (6.7-20 µm wavelength). There is significant interest in realizing cheaper and smaller spectrometers based on waveguide integrated photonics. Here we demonstrate Ge-on-Si waveguides operating up to 11 µm wavelength with low propagation loss (~ 1 dB/cm). The performance of the waveguides is then demonstrated by measuring thin films that are used to calibrate the modal overlap for molecular sensing. Lastly, an ultra-broadband Ge-on-Si waveguide polarization rotator is presented. The fabricated polarization rotator devices demonstrate a polarization extinction ratio of ≥ 15 dB over a 2 µm bandwidth (9-11 µm wavelength) with an average insertion loss < 1 dB.

Keywords: Silicon photonics, germanium waveguides, mid-infrared, molecular sensing, polarization control.

1. INTRODUCTION

The mid-infrared (MIR) part of the electromagnetic spectrum is where a vast array of molecules exhibit fundamental vibrational absorption modes, which provide unique signatures especially in the 6.7 to 20 µm wavelength region [1]. These ‘fingerprints’ allow the identification of chemical compounds with high specificity and is of particular interest for a number of applications such as environmental monitoring, healthcare, and security [2]. There has recently been significant interest into developing a MIR spectrometer based on photonic integrated circuits to significantly reduce both size and cost. Approaches based on silicon-photonics are to be preferred, since production could take advantage of existing computer chip foundries. The Ge-on-Si waveguide platform is as an excellent candidate since it could provide low loss guiding from 2 to 15 µm wavelength [3]. This platform has already demonstrated several sensing components in the MIR such as light emitters [4], plasmonic antennas [5], intersubband photodetectors [6] and third harmonic generation [7].

In this work, Ge-on-Si waveguides operating up to 11 µm wavelength with low propagation loss (~ 1 dB/cm) are demonstrated and the potential loss mechanisms at these wavelengths are discussed. Next, waveguide spectroscopy is demonstrated in the molecular fingerprint regime, by spin coating thin films of polymethyl methacrylate (PMMA) resist. The absorption coefficients of PMMA are measured to enable an experimental calibration of the optical overlap of the Ge-on-Si waveguides to predict sensing performance. Lastly, a waveguide spectrometer architecture with integrated quantum cascade lasers (QCL) is proposed. Since a QCL is a vertically linearly polarized emitting laser it will only couple to transverse magnetic (TM) waveguide modes. A waveguide polarization rotator would provide polarization flexibility. Here we demonstrate the design, fabrication and characterization of a Ge-on-Si waveguide polarization rotator operating between 9 and 11 µm wavelengths with a low insertion loss (< 1 dB) and a high polarization extinction ratio (> 15 dB).

2. Low Loss Ge-on-Si Waveguides

Ge epitaxial layers of 2 µm thickness were grown at IQE Silicon by reduced pressure chemical vapor deposition on 150 mm diameter Si (001) Czochralski substrates. The starting substrate is an important consideration since free-carrier absorption at these wavelengths is non-negligible even for relatively low background doping densities. To minimize FCA, n-type Si substrates with an electrical resistivity in the range of 10 - 20 Ω-cm, corresponding to a doping concentration of $N_D \leq 5\text{x}10^{14}$ cm^{-3} were utilized. Ge-on-Si rib waveguides were patterned by electron beam lithography using hydrogen silsesquioxane resist and dry etched by 1 µm using a mixed gas process (SF_6/C_4F_8). A waveguide width of 4 µm was chosen as this provides single mode operation over 7.5 to 11.5 µm. The waveguide losses were measured using an experimental setup previously described [8]. The Fabry-Perot fringe contrast technique was utilized to calculate the losses. To observe the Fabry-Perot fringes the effective index of the waveguide mode was tuned via the thermo-optic effect. The maximum temperature range for the measurement was limited by the thermal expansion of the stage, which caused optical misalignment of the waveguide with respect to the input and output objectives resulting in an observable slope in the measurement. The waveguide losses are lower than 5 dB/cm for both TE and TM polarization across the full measurement range (see Fig. 1). From 10 to 11 µm wavelength the TE losses reach as low as ~ 1 dB/cm [8].

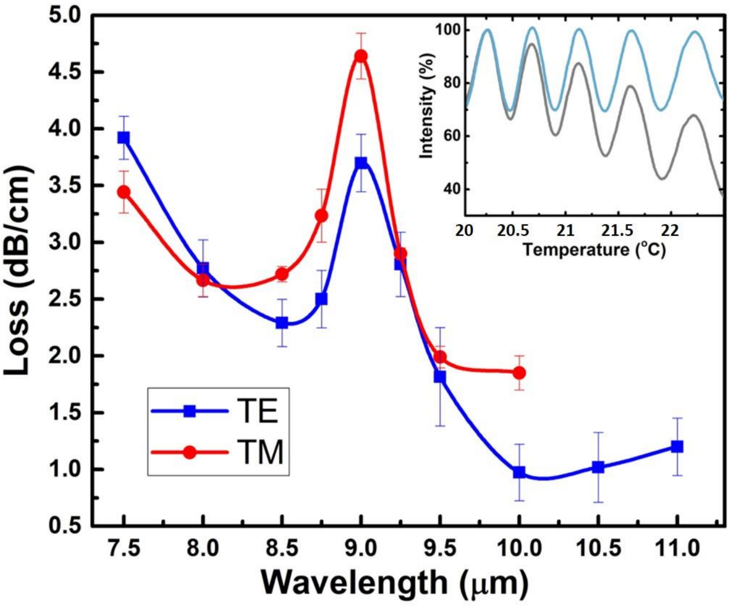

__Figure 1.__ The propagation losses measured from a 4 µm wide Ge-on-Si rib waveguide for both transverse electric (TE) and transverse magnetic (TM) polarizations. The error bars denote the standard deviation of the losses calculated by successive Fabry-Perot fringes in the transmission measurement. The inset shows the measured Fabry-Perot fringes and the drift in alignment due to thermal expansion of the stage, producing a slope in the raw data, which is subsequently corrected.

There is a noticeable trend of lower loss with increasing wavelength, which is indicative of sidewall scattering. If this is the dominant loss mechanism it has been previously shown that oxidation of waveguide sidewalls can reduce roughness, however with thermal Ge oxide, it would have to subsequently be stripped as it is not transparent in the MIR [9]. In terms of reducing the loss caused from the overlap with the Si substrate there are multiple approaches that can be taken. Thicker Ge epitaxial layers will provide greater modal confinement. The dominant loss mechanism in the Si substrate between 8 and 15 µm wavelength is absorption from an interstitial oxygen defect state at ~ 9 µm, which can be eliminated by using Float Zone Si substrates.

3. Molecular Waveguide Spectroscopy

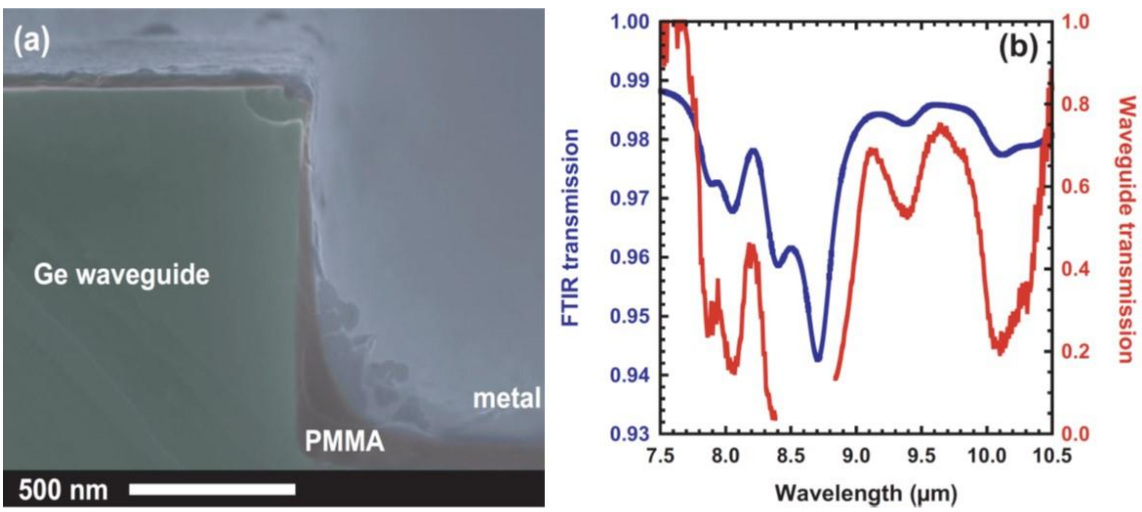

__Figure 2.__ (a) A SEM image of a Ge-on-Si rib waveguide with a thin layer of PMMA spun on top to undertake spectroscopy. The metal on top was sputtered coated before the SEM image was taken to reduce charge build up in the SEM and allow the thickness of the PMMA to be determined. (b) The FTIR transmission spectra of PMMA in blue compared to the transmission spectra of the waveguide coated with PMMA.

To demonstrate molecular absorption and vibration sensing using the Ge on Si waveguides, PMMA was spin coated onto the waveguides and the transmission was measured (see Fig. 2). An oxygen plasma was used in conjunction with a shadow mask to pattern a 1 mm long strip of PMMA over the waveguides. The results in Fig. 2 are compared to transmission results from FTIR transmission measurements. The C-O-C vibration stretching modes are clearly visible at 8.39 µm and the skeletal C-C vibration at 9.38 µm. The larger absorption from the waveguide samples is related to the longer effective propagation length through the PMMA analyte from the evanescent coupling of the mode with the analyte. This demonstrates that despite an optical overlap of < 2 %, the waveguide geometry allows for enhanced interaction with the analyte due to the increased optical path length. In the limit of weak absorption (waveguide dominated losses), the maximum sensitivity is achieved with a waveguide of length of $1/\alpha$, where α is the waveguide loss in cm^{-1}. Therefore, with 1 dB/cm propagation loss and an optical overlap of 1.2 % this provides a maximum interaction path length of ~ 520 µm. This path length would be sufficient to measure ammonia at less than part per million concentrations in the breath [10].

4. Ge-on-Si Waveguide Polarization Rotator

A waveguide spectrometer requires the integration of a source and detector along with the passive waveguides for sensing. A potential candidate for the source is a QCL since it has recently achieved significant tuning ranges. By integrating several QCLs on-chip with tunable waveguide resonators this would enable scanning across many molecular absorption lines with high power and would compensate for a non-cryogenically cooled detector. One drawback of a QCL is the inherent emitted vertical polarization that will only couple to TM guided modes. To provide polarization design flexibility a broadband waveguide polarization rotator was demonstrated. The waveguide polarization rotator is based on the mode evolution approach.

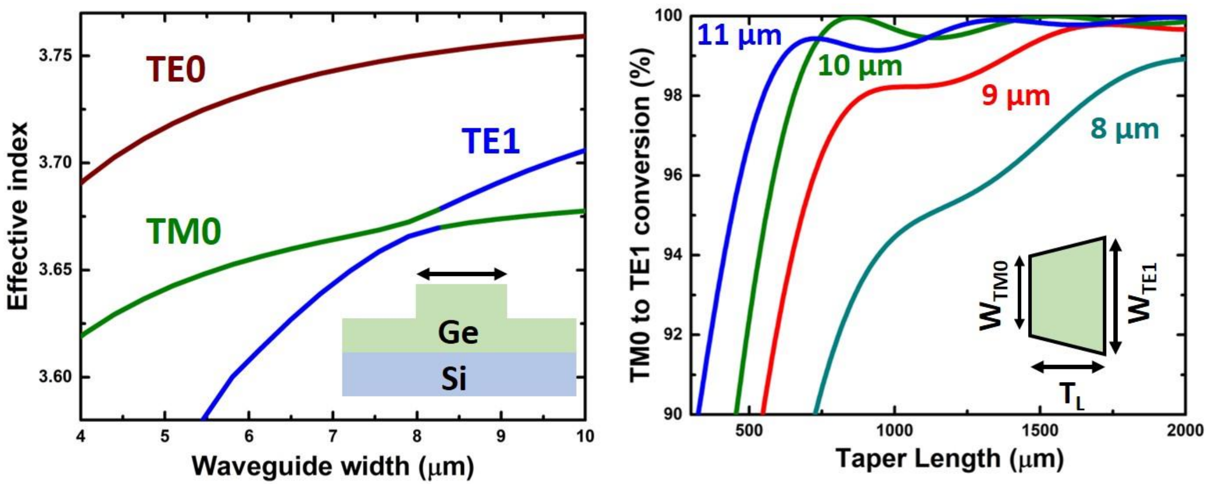

Figure 3. *(Left) The calculated modal indices versus the waveguide width for a Ge-on-Si rib waveguide at 8 µm wavelength. (Right) The modelled TM0 to TE1 mode conversion efficiency versus taper length for an input width of 7.7 to an output width of 8.7 µm, at 8, 9, 10 and 11 µm wavelength.*

A finite-difference eigenmode solver was used to calculate the supported eigenmodes versus the waveguide width of a 2 µm thick Ge-on-Si rib waveguide with a partial 1 µm etch. It is clear from Fig. 3 (Left) that there is an anti-crossing between the TM0 and TE1 modes at a waveguide width of ~ 7.9 µm, which is indicative of mode hybridization. To enable broadband TM0 to TE1 mode conversion from 8 to 11 µm wavelength requires a taper design that has an input and output width that covers the mode hybridization points at the wavelength extremes. An eigenmode expansion solver (EME) was used to model a linear taper with an input and output width of 7.7 and 8.7 µm, respectively. The calculated TM0 to TE1 polarization conversion efficiency (PCE) for different wavelengths versus taper length is shown in Fig. 3 (right). It is clear that for a 2 mm long taper there is a PCE of > 99 % over the full wavelength range.

To provide broadband TE1 to TE0 conversion the higher-order mode converters proposed by D.Chen et al. were utilized [11]. This asymmetric taper structure was optimized using EME and a particle swarm algorithm for a centre wavelength of 9.5 µm. Figure. 4 (Left) shows that after optimization, close to 80 % conversion over a 2 µm bandwidth (9- 11 µm) is achieved. A waveguide polarization rotator consisting of a 2 mm long linear taper for broadband TM0 to TE1 mode conversion followed by the optimized TE1 to TE0 higher order mode converter were microfabricated and experimentally characterized using previously described techniques [1]. A high extinction ratio (≥ 40 dB) wire grid polarizer was used to ensure only a TM fundamental mode was excited at the input. At the output, the polarization axis of another identical polarizer was adjusted for the detection of the transmitted TE0 and TM0 modes by recording each spectrum on a mercury cadmium telluride detector. The ratio of these provides the polarization extinction ratio. The insertion loss was measured by comparing the transmittance of eight reference straight waveguides that had the same overall length. The fabricated device demonstrates a polarization extinction ratio of > 15 dB and an insertion loss of < 1 dB over the 9-11 µm wavelength region (see Fig. 4 (Right)) [12].

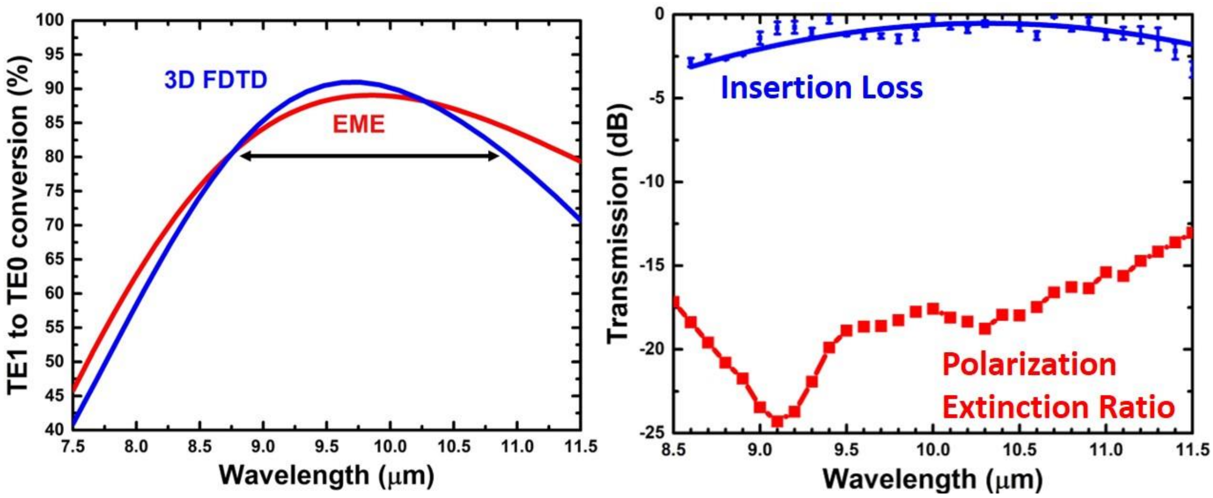

Figure 4. *(Left) The TE1 to TE0 mode conversion efficiency for the optimized higher order mode converter consisting of six asymmetric tapers modelled with the EME solver and 3D FDTD. (Right) The experimentally measured polarization extinction ratio and insertion loss as a function of the wavelength.*

5. CONCLUSIONS

We have experimentally measured the propagation loss of Ge-on-Si rib waveguides and demonstrate losses as low as ~ 1 dB/cm at 11 µm wavelength. These waveguides were used to demonstrate spectroscopy of PMMA with C-O-C and C-C vibrational absorptions clearly visible. Lastly a broadband Ge-on-Si waveguide polarization rotator that operates between 9-11 µm wavelength with a low insertion loss (< 1 dB) and a high polarization extinction ratio (> 15 dB) was demonstrated.

REFERENCES

1. Hollas, J.M., *Modern spectroscopy*. 4th ed. 2004, Chichester ; Hoboken, NJ: J. Wiley. xxvii, 452 p.
2. Baldassarre, L., et al., *Midinfrared Plasmon-Enhanced Spectroscopy with Germanium Antennas on Silicon Substrates.* Nano Letters, 2015. **15**(11): p. 7225-7231.
3. Soref, R., *Mid-infrared photonics in silicon and germanium.* Nature Photonics, 2010. **4**(8): p. 495-497.
4. Millar, R., et al., *Mid-infrared light emission> 3 µm wavelength from tensile strained GeSn microdisks.* Optics express, 2017. **25**(21): p. 25374-25385.
5. Pellegrini, G., et al., *Benchmarking the use of heavily doped Ge for plasmonics and sensing in the mid-infrared.* ACS Photonics, 2018. **5**(9): p. 3601-3607.
6. Gallacher, K., et al., *Mid-infrared intersubband absorption from p-Ge quantum wells grown on Si substrates.* Applied Physics Letters, 2016. **108**(9): p. 4.
7. Fischer, M.P., et al., *Plasmonic mid-infrared third harmonic generation in germanium nanoantennas*. Light: Science & Applications, 2018. **7**(1): p. 106.
8. Gallacher, K., et al., *Low loss Ge-on-Si waveguides operating in the 8-14 um atmospheric transmission window.* Optics Express, 2018. **26**(20): p. 25667-25675.
9. Pezzoli, F., et al., *Disentangling nonradiative recombination processes in Ge micro-crystals on Si substrates.* Applied Physics Letters, 2016. **108**(26): p. 262103.
10. Griskeviciute, U., et al., *Ge-on-Si waveguides for sensing in the molecular fingerprint regime.* Optics Express, 2020. **28**(4): p. 5749-5757.
11. Chen, D.G., et al., *Low-loss and fabrication tolerant silicon mode-order converters based on novel compact tapers.* Optics Express, 2015. **23**(9): p. 11152-11159.
12. Gallacher, K., et al., *Ultra-broadband mid-infrared Ge-on-Si waveguide polarization rotator.* APL Photonics, 2020. **5**(2): p. 026102.