MEMS-Enabled On-Chip Computational Mid-Infrared Spectrometer Using Silicon Photonics

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Cite This: https://doi.org/10.1021/acsphotonics.2c00381

ABSTRACT: On-chip spectrometers using silicon photonics offer a compact, energy-efficient, and cost-effective solution to biochemical spectroscopy and hyperspectral imaging in integrated and portable application scenarios. The mid-infrared (MIR) spectral band is critical to spectroscopic sensing. However, the existing on-chip spectrometer approaches are limited in the MIR. Here, we present an on-chip computational spectrometer in MIR (3.7–4.05 μm) using an MEMS-enabled silicon photonic integrated device, which is realized via the time-domain modulation of reconfigurable waveguide couplers. The electrostatically actuated on-chip spectrometer intrinsically features low power consumption and single-pixel detection and offers multiplexing advantages, potentially leading to a high signal-to-noise ratio. We achieve laser spectrum reconstruction across a large bandwidth (350 nm) experimentally. Furthermore, based on a linear superposition assumption, we achieve the polychromatic light reconstruction of narrow spectral features (3 nm resolution) and a broad absorption spectrum of nitrous oxide gas using a regularized regression method.

KEYWORDS: MIR photonics, photonic integrated circuit, reconfigurable photonics, optical MEMS, on-chip spectrometer

INTRODUCTION

Optical spectrometers are among the most widely used types of experimental instruments for biochemical sensing and material analysis.1 In the past decades, there has been a rapid increase in the use of spectrometer systems in many academic and industrial areas, including precision agriculture, environmental monitoring, marine science, and food industry.2 In these application scenarios, the spectroscopy analysis is often expected to be instantaneous on the site, which leads to the development of miniaturized optical spectrometers.3–7 Among them, silicon photonics is one of the most promising technologies. Leveraging the advantages of CMOS compatibility and integration, the chip-scale spectrometers based on photonic integrated circuits (PIC) can be compact and of low cost.8,9

To date, most on-chip spectrometers based on PICs rely on planar dispersive gratings,10–14 narrowband filters,15,16 and Fourier transform (FT) interferometers.17–21 Besides, some approaches are using computational reconstruction.22,23 On-chip spectrometers based on dispersive elements and narrowband filters can provide a high resolution by spectral channel division. However, signal-to-noise (SNR) could be a problem for these devices since light is split into many spectral channels. What is more, the multichannel architecture often requires a corresponding detector array, which increases the footprint, cost, and complexity of the PICs. Compared to these systems, FT spectrometers have some inherent advantages, known as the multiplexing advantage (Fellgett’s advantage) and high optical throughput (Jacquinot’s advantage). Thus, it brings a high SNR to FT spectral analysis. With reconfigurable components in PIC circuits, an on-chip FT spectrometer can be implemented with a single-pixel detector and digitalized control. Combining the thermo-optic tuning and Mach–
Zehnder interferometer (MZI) waveguide architecture, researchers have demonstrated on-chip FT spectrometers working around 1550 nm wavelength with good performances (resolution below nanometer and bandwidth of tens of nanometers).17,19,21 However, despite the work demonstrated in the near-infrared wavelength range, investigations on on-chip spectrometers might not be adequate in the MIR wavelength range (typically defined as 2−20 μm).24−28 The MIR range contains strong characteristic absorption bands of many biochemical molecules. The so-called fingerprint region is of great interest to spectroscopy sensing.29,30 The MIR on-chip spectrometer can play an important role in lab-on-a-chip applications.31 Prior work in MIR has mainly demonstrated the FT spectrometer based on discrete MZIs.24−27 The spatial heterodyne spectrometer design relies on the number of discrete MZIs to increase its spectral resolution, which demands a high-cost detector array and could result in an excessive footprint. To further develop on-chip applications in MIR, reconfigurable photonics are desired to empower on-chip optical functionalities. Recent years have seen growing interest in reconfiguration in MIR PICs.32 The reconfiguration mechanisms, including mechanical motion, free carrier injection, thermo-optic tuning, and so forth, have been demonstrated in the MIR region. Among these approaches,32 optical MEMS on a silicon-on-insulator (SOI) platform could be an auspicious choice for the MIR reconfigurable photonics. With the removal of the buried oxide (BOX) layer, mechanical motion of the on-chip photonic waveguide can be enabled. Meanwhile, the optical loss induced by BOX in the MIR region can be eliminated, thus sustaining the competitiveness and cost-effectiveness of SOI technology. Additionally, reconfiguration using electrostatic actuation could offer an energy-efficient, low-loss, and effective approach to the MIR on-chip optical systems.36 Thus, the MEMS-enabled silicon PIC device could be a promising solution to the high-performance on-chip spectrometer in the MIR.

In this paper, we experimentally demonstrate an MIR on-chip silicon MEMS-enabled computational spectrometer (Si-McS) working around a wavelength of 4 μm, which is accomplished using a pair of simple MEMS tunable waveguide couplers on an SOI platform. The proposed Si-McS concept brings inherent FT advantages to the on-chip spectroscopy, ensuring a high SNR and requiring a single-pixel photodetector only. Moreover, the presented MEMS-reconfigurable approach shows superior performance for on-chip reconfiguration photonics in the MIR SOI platform (see Supporting Information Note 8). It breaks SOI’s limitation in the MIR region and potentially facilitates chip-level integration by fully leveraging the infrastructures built on SOI platforms. These contribute to the high performance and compactness of the demonstrated Si-McS in MIR (see Supporting Information Note 8). The effective tuning of the waveguide couplers can be realized using electrostatic actuation in our 3D heterogeneous...
integrated device. The spectra can be acquired via the time-domain actuation of the MEMS tunable waveguide couplers. We implement machine learning-regularized regression methods to computationally reconstruct the spectra. We experimentally demonstrate the sparse spectrum reconstruction of laser peaks on every 1 nm over a 350 nm bandwidth (3.7–4.05 μm). Based on a linear superposition assumption on detector response, we carry out polychromatic spectrum reconstruction using laser measurement results. Double-wavelength reconstruction results show a 3 nm resolution of the proposed Si-McS device. Moreover, a gas cell inflated by nitrous oxide (N₂O) gas is placed into the experimental setup for antireflection (OPD). In the proposed concept, OPD modulation is obtained by active time-domain modulation of the coupling strength between photonic waveguides. The suspended silicon waveguide with SWG claddings are demonstrated spectroscopy system is shown in Figure 1a.

**RESULTS**

**Si-McS Architecture.** The concept of the Si-McS is analogous to Fourier transform infrared spectrometer (FTIR), which relies on the modulation of the optical path difference (ODP). In the proposed concept, ODP modulation is obtained by active time-domain modulation of the coupling strength between photonic waveguides. The suspended silicon waveguide is designed to be a single mode with TE polarization. It is known that the coupling between a pair of waveguides can be understood as the interference between the formed two supermodes in the waveguide coupler, namely, symmetric mode (SM0) and asymmetric mode (SM1). Considering the effective index difference between SM0 and SM1 (Δn(ℏ) = n₁(ℏ) − n₂(ℏ)), the interference can be observed at the output through and drop ports after these two modes propagate through a given coupling length. Thus, interferograms can be generated at either output port by time-domain tuning of the coupling strength of a waveguide coupler with a certain coupling length, which is similar to the modulation of ODP. In our prior work, we briefly elaborate on the working principle of a discrete design with simulation results. Here, we introduce our architecture on an MIR silicon photonics platform with a continuous tuning of a fixed-length waveguide coupler. In the aspect of photonics design, suspended waveguide with subwavelength grating (SWG) claddings on the SOI platform is adopted by considering easy integration between the MEMS actuator and MIR photonics waveguide (see Figure 1b insets). The waveguide coupler is formed by two silicon strip waveguides with single-side SWG claddings. Waveguide claddings are converted from the single side to the double side to define the movable and stationary regions, as shown in Figure 1b. In the aspect of MEMS design, as shown schematically in Figure 1c, the MEMS cantilever can be electrostatically actuated upward using our 3D heterogeneous integration method. In such an architecture, coupling strength between these two photonic waveguides can be reconfigurable through adjusting the vertical gap. From our simulation results (Figure 1d), adjusting the vertical gap offers a convenient way for tuning the effective index difference Δn(ℏ). Details of the waveguide study can be found in Supporting Information Note 1. We can choose either the through port or drop port of the waveguide coupler as the output and we can actively adjust the vertical gap to measure the interferogram at the output, thus enabling the acquisition of the light spectrum. The propagation loss and bending loss of the suspended silicon waveguide with SWG claddings are measured to be ~2.9 dB/cm and ~0.076 dB each (Supporting Information Note 1). The response time of the MEMS cantilever actuator is estimated to be 11.5 μs (Supporting Information Note 3). The device footprint is 4.5 mm × 0.6 mm, which includes a pair of reconfigurable photonic waveguide couplers.

For a directional coupler with a certain coupling length L, the output power from the through and drop ports can be described as

\[
P_{\text{through}}(L, λ) = B(λ)\cos^2\left(\frac{πL}{λ}Δn\right)
\]

(1)

\[
P_{\text{drop}}(L, λ) = B(λ)\sin^2\left(\frac{πL}{λ}Δn\right)
\]

(2)

where \(P_{\text{through}}\) and \(P_{\text{drop}}\) are the output light power at the corresponding ports, \(B\) is the spectrum of input light, \(λ\) is the light wavelength, and \(Δn\) is the effective index difference between SM0 and SM1. It is well-known that the interferogram of a Michelson interferometer in a traditional FTIR can be given as

\[
I_D(x, λ) = 0.5B(λ)\left(1 + \cos\left(\frac{2πx}{λ}\right)\right) = B(λ)\cos^2\left(\frac{πx}{λ}\right)
\]

(3)

where \(x\) is the OPD and \(I_D\) is the output power of the interferometer. From eqs 1–3, it can be found that the analogous ODP offered by the Si-McS can be understood as \(x = LΔn\). More specifically, in the operation of the Si-McS, we can use a time-domain bias voltage \((V_{\text{bias}})\) signal on the MEMS actuator to adjust the vertical coupling gap (h) between the waveguides, thus realizing the time-domain modulation of \(Δn\) step by step. To further clarify the intrinsic FT mechanism of the proposed device with the fact that \(Δn\) is a function of both \(h\) and \(λ\) taken into consideration, \(Δn(ℏ, λ)\) is approximated by a polynomial function

\[
Δn(ℏ, λ) ≈ f_2(ℏ)f_2^*(ℏ) = (a_1 + a_2ℏ)(b_1 + b_2ℏ + b_3ℏ^2 + b_4ℏ^3)
\]

(4)

which is validated using numerical calculations (see Supporting Information Note 2). Given the device geometry, the polynomial approximation can be fitted with a 99.5% R-squared value.

Furthermore, combining eqs 1 and 4, the output power of the through port in the proposed spectrometer can be given as

\[
P_{\text{through}}(x_i, u) = B(u)\cos^2\left(\frac{πL}{λ}Δn(ℏ, λ)\right) = B(u)\cos^2\left(\frac{πL}{λ}f_2(ℏ)f_2^*(ℏ)\right) = B(u)\cos^2\left(πux_i\right)
\]

(5)

where the effective wavenumber and ODP are defined as \(u = f_2(ℏ)/λ = (a_1 + a_2ℏ)/λ\) and \(x_i = Lf_2(ℏ)\), respectively. Therefore, \(B(u)\) can be achieved by performing an FFT of the interferogram \(P_{\text{through}}\). With \(λ = a_1/(u - a_2)\), the spectrum \(B(λ)\) can be obtained by mapping the effective wavenumber \(u\) to the wavelength \(λ\). The eqs 4 and 5 highlight the conceptual
working mechanism of the Si-McS using an MEMS-tunable directional coupler. In our demonstrations, considering the fact that functions $f_1$ and $f_2$ are difficult to be precisely determined experimentally, we used a regularized regression model for computational spectrum reconstruction instead.

Experimental Device. We experimentally validated the Si-McS concept in the MIR region using our 3D assembled photonic MEMS device. The experimental device consists of a glass chip (500 $\mu$m thick) on top and an SOI MEMS PIC chip (500 nm-thick device layer and 2 $\mu$m-thick BOX) at the bottom. The optical waveguides are fabricated on an SOI wafer using a foundry-compatible silicon photonics process.

The gold-patterned glass chip is aligned and bonded on the SOI chip via aluminum (Al) solder by flip-chip bonding, providing the top electrode for electrostatic actuation. This 3D integration approach offers a large tunable range for the MEMS cantilevers, thus enabling the effective tuning of the waveguide coupler. As shown in Figure 2b, the Al solders also work as the electrical interconnect between the top and bottom chips. With insulation trenches on the SOI chip, we can apply bias voltage to the top electrode on the glass chip via the electrical input on the SOI chip, which facilitates the Si-McS operation. The optical input and output are achieved via the fiber-to-chip grating couplers. Here, we choose a narrow coupling gap of 200 nm for the waveguide coupler (Figure 2a), which depends on our current nanofabrication capabilities. To validate the concept, we choose a long coupling length of 7680 $\mu$m, which is offered by two cascaded waveguide couplers (shown in Figure 2c,d). A longer coupling length could lead to a finer spectrometer resolution. Here, we estimate the theoretical resolution based on the Rayleigh criterion, Supporting Information Note 4), and choose a coupling length of 7680 $\mu$m which is promising for our experimental demonstration. Besides, the coupling length is chosen to be the integral multiple of the SWG period to well integrate the waveguide design. The two MEMS cantilevers are electrically grounded and actuated simultaneously by a top electrode covering both of them (Figure 2b). We use the design of two MEMS cantilevers here to achieve design compactness. Considering an MEMS cantilever length of 85 $\mu$m and an initial air gap of 12 $\mu$m, the pull-in voltage of the electrostatic actuation can be estimated to be 140 V.39

Before we proceed to the experimental validation of the Si-McS, we carry out a characterization process to test the

![Figure 2](a) SEM image of the waveguide coupling region. (b) A-A' section view of the 3D assembled device. (c) SEM image of the movable waveguide coupler. (d) Optical microscopy image of the MEMS actuation region of the device.

![Figure 3](a) Experimental setup for the MIR reconfigurable photonics device characterization. (b) Calibrated measurement matrix $D$ of the on-chip spectrometer. The wavelength range is swept in a 1 nm high resolution, and 71 steps of DC bias voltage are gradually applied to the MEMS actuator.
electrostatic actuation voltage using a photonic switch design on the same chip (see Supporting Information Note 3). This could help us understand the decoupling condition of the reconfigurable waveguide coupler and the pull-in voltage of the MEMS cantilever. The experimental setup for this device characterization is depicted in Figure 3a. An MIR tunable laser is used as the single-wavelength light source. The optical input/output to the Si-McS is achieved using fiber-to-chip grating couplers. Depending on the transmission bandwidth of the grating coupler, we carry out the optical testing in the wavelength range between 3.7 and 4.05 μm. From the voltage testing results in Supporting Information Note 3, it can be found that the resonance frequency of the MEMS actuator is 87 kHz (roughly corresponds to an 11.5 μs device response time) and 80 V bias voltage is sufficient to actuate the waveguide coupler from a fully coupled to a decoupled condition. To simplify the experimental implementation and compensate for the fabrication imperfections of the on-chip device, we adopt a computational scheme to reconstruct the spectrum with the use of the machine learning regression method. We choose a time-sequenced bias voltage from 0 to 80 V to acquire the interferogram. The bias voltage sequence is applied by a 2 V interval between 0 and 20 V gradually followed by a 1 V interval from 20 to 80 V, which is a total of 71-step bias voltage. A larger voltage increase is chosen at lower bias because the optical response is relatively small below 20 V bias voltage (see the actuation calibration results in Supporting Information Note 3).

Next, we work on the demonstration of the Si-McS spectrum reconstruction using the depicted setup (Figure 3a). At the first step, we work on the calibration of the computational reconstructive Si-McS. The output intensities from the drop port of the Si-McS are collected with a step-by-step increase of bias voltage (71 steps) applied at each wavelength between 3.7 and 4.05 μm with an increase of 1 nm. These calibration intensity data form matrix $A (m \times n)$, indicating the spectral response of the device in the current testing system. Each column of $A$ represents specific intensity outputs of the Si-McS generated at the corresponding light wavelength and includes 71 optical intensity points ($m = 71$) under the time-domain MEMS actuation. A total of 351 columns correspond to the swept wavelength points ($n = 351$) by the MIR tunable laser. In the experimental testing setup, the testing system has a wavelength-dependent feature caused by the tunable laser output, grating coupler efficiency, and detector spectral response. The optical transmission through a straight waveguide on the same chip, which comprises the same wavelength-dependent testing system feature, is measured and regarded as the reference input light intensity. The laser swept spectrum passing through the straight waveguide is recorded as a vector $G = [g_1, g_2, \ldots, g_n]^T$ with 351 elements. Thus, the calibrated measurement matrix $D (m \times n)$ of the on-chip spectrometer can be given as

$$D = A \cdot \text{diag} \left( \frac{1}{g_1}, \ldots, \frac{1}{g_n} \right)$$

(6)

where diag represents the diagonal matrix form. Once the measurement matrix $D$ is calibrated, it remains fixed if the system is unchanged and can be used to retrieve the light spectrum directly. For an arbitrary incident light spectrum $S$ (a column vector with 351 elements), the interferogram $I$ measured by the detector is

$$I = DS$$

(7)

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Figure 4. Single-wavelength spectrum reconstruction. (a) Reconstructed laser lines (gray lines) showing the original solutions of $S$ by the elastic-net method (training sets in blue and reference intensity in orange). (b) Measured interferograms at several different laser wavelengths. (c) Corresponding reconstructed spectra from the interferograms shown in (b).
where I is a column vector with 71 elements. Each element represents the optical output intensity at a certain bias voltage. As the calibrated measurement matrix D used in our system is in a size of 71 × 351 (shown in Figure 3b), we use the regularized regression techniques to solve the underdetermined equation to determine the incident spectrum S. To properly solve the sparsity signal and account for system robustness, we choose the regularized regression model including both L1-norm and L2-norm, namely, the elastic-net. It solves the regularized regression problem

$$\min_{\hat{S}} \left\{ ||I - DS||^2 + \alpha_1 ||S||_1 + \alpha_2 ||S||^2 \right\}$$

(8)

where two regularized weights (hyperparameter $\alpha_1$ and $\alpha_2$) are applied to the L1-norm and L2-norm of the solution (S vector), respectively. In this study, we adopt scikit-learn to implement it in Python.40

**Single-Wavelength Reconstruction.** To achieve appropriate hyperparameters for our Si-McS characteristics, we implement a machine learning approach for grid search for $\alpha_1$. For reconstruction of single-wavelength spectra, we manually adjust the hyperparameter $\alpha_1$ to zero by considering the signal’s extreme sparsity. For grid search of the hyperparameter $\alpha_1$, we measure the interferograms at 34 wavelengths using time-domain MEMS actuation. These wavelengths are evenly chosen across the whole operation wavelength band (Figure 4a). These 34 measured interferograms form the training sets $I_j$ (j = 1, 2, ... 34), where each I is a column vector with 71 elements. By solving the regularized problem, we can obtain the corresponding incident spectrum $S_j$. As the tunable MIR laser has a linewidth of 0.2 nm, we take the reference incident laser spectrum as a column vector $S_1$ with high sparsity that has only one nonzero intensity value taken from the measurement $G = [g_1, g_2, \ldots, g_n]^T$. For example, given a laser input from the ith wavelength $\lambda_i$, only $S_1(i)$ equals $G(i)$ and all the other elements in $S_1$ are zero. We carry out the grid search in the 34 training sets to choose $\alpha_1$ that minimizes the total mean squared error (MSE) between the solution $S_j$ and $S_1$. The total MSE is calculated by

$$\sum_{j=1}^{34} \left\{ \frac{1}{n} \sum_{i=1}^{n} (S_j(i) - S_1(i))^2 \right\}$$

(9)

From the grid search in the training set, the optimal $\alpha_1$ is determined to be $3.79 \times 10^{-4}$. The determined hyperparameter $\alpha_1$ represents an intrinsic characteristic of the on-chip Si-McS. Thus, it is consistently applied to the following spectrum reconstruction. Next, we use the hyperparameters ($\alpha_1 = 3.79 \times 10^{-4}$ and $\alpha_2 = 0$) to predict the incident laser wavelength across the spectral range (3.7–4.05 μm) (Figure 4a). An interferogram $I$ is collected at each selected wavelength, and it is used to solve the regularized problem for the incident spectrum $S$. The remaining 317 recorded interferograms form the test sets with their reconstructed laser spectra are presented in gray where the 34 training sets are denoted in blue. The reference intensity $G$ is plotted as a continuous line in orange. It is noted that the intensity dip around a wavelength of 3.8 μm is caused by the nonuniform MIR laser output. A few reconstructed laser spectra that do not belong to the training sets are chosen to further demonstrate the high-performance reconstruction (Figure 4c), and their corresponding interferograms are shown in Figure 4b. The regression model training and prediction results are summarized in Table 1. The low level of MSE ($10^{-4}$) in the testing sets proves that the adopted machine learning regression method is valid to be used on the Si-McS spectrometer for sparse signal reconstruction. Over the whole working wavelength range (350 nm bandwidth), the laser wavelengths can be precisely reconstructed within ±1 nm accuracy.

**Double-Wavelength Reconstruction.** Due to the lack of polychromatic MIR light sources in our laboratory, we use the following scheme to emulate the experimental polychromatic interferometers using a tunable laser source. Assuming a polychromatic light source with a known spectrum containing a total of n number of wavelength components, the tunable laser is tuned to each wavelength component with its intensity properly set, and its interferogram $I_h$ ($h = 1$ to $n$) from the Si-McS is recorded. Assuming that the detector response is proportional to the linear superposition of all intensities at those wavelength components at the detector, the experimental interferogram ($I_p$) by a polychromatic input containing n wavelength components can be given as a summation of all $I_h$ recorded

$$I_p = \sum_{h=1}^{m} I_h$$

(10)

Under this scheme, we reconstruct the polychromatic spectrum using the experimental interferogram $I_p$. Further discussion on the validation of the linear superposition assumption can be found in Supporting Information Note 5. Two tunable laser sources working in the near-infrared wavelength range are adopted in the testing of a waveguide coupler device. The measured output optical intensity by simultaneously injecting two wavelengths equals approximately to the summation of the individually measured optical intensities when each wavelength is injected alone. This is valid during our multistesting with different combinations of wavelengths and input powers. It could be ideal to use an additional MIR laser or a broadband MIR light source to carry out the experiments. However, with the lack of an extra MIR laser or a commercially available MIR broadband light source in the laboratory, we evaluate the proposed Si-McS performance under the well-validated linear superposition assumption and a single tunable MIR laser.

We carry out the spectrum reconstruction on the polychromatic input consisting of two laser lines to determine the spectral resolution of the Si-McS under the adopted computational scheme. In the first step, we obtain the experimental interferogram $I_p$. Given the reconstruction for $\Delta\lambda = 2$ nm as an example, we first measure the interferograms $I_1$ ($71 \times 1$) and $I_2$ ($71 \times 1$) at wavelengths of 3.900 and 3.902 μm, respectively. The experimental interferogram $I_p$ generated by a polychromatic light source containing these two wavelengths (3.900 and 3.902 μm) is given as $I_p = I_1 + I_2$. Next, we use $I_p$ and the same calibrated measurement matrix (D) to solve the regularized regression problem to specify the

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<th>Table 1. Model Fitting and Prediction Results for Laser Lines Using the Elastic-Net Method ($\alpha_1 = 0$)</th>
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<td><strong>number of</strong></td>
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Considering the sparsity of the polychromatic input, we adopt the elastic-net method and the same hyperparameters ($\alpha_1 = 3.79 \times 10^{-4}$ and $\alpha_2 = 0$) as those used in the previous section to solve the problem. It can be found that the wavelength and intensity features of the spectra can be well reconstructed (Figure 5a). The reference intensity shown in Figure 5 is taken from the measurement intensity vector $G$. The spectral resolution of the Si-McS is determined by the minimum resolvable spacing between the two laser lines. In our experiments, a 2 nm resolution can be barely obtained (Figure 5b) and a 3 nm resolution is achieved (Figure 5c), which exceeds the Rayleigh criterion (Supporting Information Note 4). Besides, we analyze the robustness of the spectrum reconstruction using the proposed algorithm with the same hyperparameter ($\alpha_1 = 3.79 \times 10^{-4}$ and $\alpha_2 = 0$). The main factor causing the degradation of the reconstruction performance could be the measurement errors from the MEMS-enabled PIC device. Here, we analyze the relative errors of two acquired interferograms at the same wavelength (see Supporting Information Note 6). Among 300 sets of measurement data, the relative errors extracted range from 1.2 to 3.1% with an average of 2.4%. Next, we numerically apply increasing noise levels to the experimental interferograms and investigate the reconstruction performances. It can be found that the spectra can be well retrieved up to a maximum of 4% relative error in the experimental interferograms. The details of the investigation can be found in Supporting Information Note 6. These results show the accuracy and repeatability of our MEMS-enabled device for the data acquisition and the robustness of spectrum reconstruction using the proposed computational technique.

**Broad Absorption Spectrum Reconstruction.** The MIR region is important for absorption spectroscopy. Here, we use the Si-McS to demonstrate the broad spectrum reconstruction for N$_2$O gas absorption spectroscopy. N$_2$O gas is a potent greenhouse gas that destructs the stratospheric ozone. The miniaturized spectroscopic instrumentations could contribute to the monitoring of N$_2$O emissions. A customized gas cell (25 cm optical length) is inserted into the current testing setup between the half-wave plate and ZnSe lens for the investigation of gas spectroscopy (Supporting Information Note 7). Thus, it is necessary to recalibrate the measurement matrix $D$ in the modified testing setup with the gas cell inserted.

![Figure 5. Double-wavelength spectrum reconstruction. (a) Reconstructed and reference polychromatic spectra comprising double laser lines with different wavelength spacings (solved using the elastic-net method with the same hyperparameters used for Figure 4). (b) Zoom-in view of the spectra with 2 nm spacing. (c) Zoom-in view of the spectrum with 3 nm spacing. Two laser lines are well-distinguished.](https://doi.org/10.1021/acsphotonics.2c00381)
We use the gas cell filled with ambient air for testing system calibration. The same time-sequenced bias voltage with 71 steps is adopted. First, we sweep the tunable laser passing through the straight waveguide with a step of 4 nm from 3.82 to 4.02 μm. The measured results $G'$ are regarded as the reference input light intensity passing through the air gas cell. Second, we retrieve the spectral response matrix $A'$. Thus, we can achieve the calibrated measurement matrix $D'$ under the current gas spectroscopy testing system using eq 6. Similarly, we still adopt the elastic-net method (hyperparameter $\alpha_1 = 3.79 \times 10^{-4}$) to implement the computational reconstruction. Considering the target broadband signal, we put a relatively large weight on the $\alpha_2$ and adjust the hyperparameter $\alpha_2 = 99 \alpha_1$ to increase the model robustness.

Next, we work on the reconstruction of light spectra passing through the air gas cell ($S_{air}$). Again, based on the linear superposition response of the Si-McS, the experimental interferogram $I_{air}$ for a polychromatic input comprising 51 wavelength elements is obtained by a summation of all the interferograms measured at each wavelength. The measured interferograms can be found in Supporting Information Note 7. The calibrated measurement matrix $D'$ and experimental interferogram $I_{air}$ are used to solve the regularized problem for the spectrum $S_{air}$. The reconstructed light spectrum passing through the air gas cell is shown in Figure 6a.

Next, we inflate the gas cell with N2O gas for gas spectroscopy demonstration. We collect the experimental interferogram $I_{N2O}$ by a polychromatic input comprising the 51 wavelength elements based on the linear superposition assumption. Measurement results of the interferograms on each wavelength can be found in Supporting Information Note 7. Thus, we solve the regularized regression problem with the calibrated measurement matrix $D'$ and experimental interferogram $I_{N2O}$. The solution $S_{N2O}$ representing the reconstructed absorption spectrum of the N2O gas cell is shown in Figure 6b. For comparison, we also send the laser through the N2O gas cell and a straight waveguide and sweep its wavelength. The laser intensity at each wavelength is recorded and denoted as $G'_{N2O}$ which serves as the reference absorption spectrum of the N2O gas cell. From the absorbance spectrum (Figure 6c), it can be found that the spectral features of the N2O gas can be well recognized. The inset in Figure 6c briefly depicts the modified testing system, and details can be found in Supporting Information Note 7.

## DISCUSSION

Considering the rapid progress in the development of MIR silicon photonics, the outstanding performance of the Si-McS can be expected. First, a superior spectral resolution of the Si-McS device can be pursued using the advanced silicon photonics foundry process. The extension of the waveguide coupler length with low-loss waveguides and the reduction of the waveguide coupling gap can lead to a finer spectral resolution based on the proposed Si-McS concept (Supporting Information Note 4). Leveraging on the advanced nano-fabrication foundry process, the narrowing coupling gap also contributes to the reduction of the device footprint. Second, the operation bandwidth of the Si-McS device can be further explored. The demonstrated bandwidth of 350 nm is limited by the available transmission bandwidth of the fiber-to-chip grating coupler. The further enhanced bandwidth might be achieved using fiber-to-chip edge couplers. Third, the adopted electrostatic MEMS actuation guarantees an extremely low energy consumption operation of the Si-McS. With the improvement of the 3D MEMS integration approach, the bonding gap between the chips can be further reduced, thus potentially lowering the operating bias voltage.

The demonstrated Si-McS using MEMS-enabled silicon photonics exhibits promising capability of the reconfigurable MIR photonic devices. The MEMS approach for MIR PIC reconfiguration extends the usage of SOI wafer to a longer wavelength in a low-loss, energy-efficient, and effective way.
which may enable multicomponent MIR spectroscopic sensing on a single chip.

To conclude, we experimentally demonstrate an on-chip-integrated spectrometer using a reconfigurable MIR silicon photonic device. The proposed Si-McS concept is discussed, which is intrinsically analogous to a Michelson interferometer and FTIR. The experimental device consists of a pair of MEMS reconfigurable silicon waveguide couplers operated at MIR wavelengths. The CMOS-compatible fabrication process and single-detector scheme potentially ensure low-cost manufacturing. In our experiments, a highly accurate (1 nm accuracy) single-wavelength spectrum reconstruction over a large bandwidth (350 nm) is experimentally achieved. Moreover, based on a linear response assumption of the detector, we carry out the spectrum reconstruction for polychromatic light. The spectral resolution of the demonstrated Si-McS is determined to be 3 nm by the double wavelength reconstruction results. The absorption spectrum of N₂O gas in the Si-McS operation window is investigated, and the spectral absorption feature of the gas is well recognized. Our study proposes a valid approach to achieve high-performance and compact MIR spectrometry on a single chip (Supporting Information Note 8). Considering the effectiveness of the MEMS reconfiguration mechanism, this concept can be applied to other wavelength bands and can also be extended to other photonics platforms besides silicon. The Si-McS can be an important building block for spectroscopy-on-a-chip applications, contributing to the miniaturized, robust, and low-cost portable spectroscopic sensors.

## METHODS

**Device Fabrication.** The proposed MIR Si-McS is fabricated using an industry-compatible process. It consists of two chips. The glass chip (0.8 × 0.8 cm²) is chosen for the top electrodes because of its insulation property. The bottom chip is a 1.5 × 1.5 cm² SOI chip. First, metal patterns, including the electrodes, bonding pads, and markers, are fabricated on the glass chip using standard optical lithography (LaserWriter, LW405b; photoresist: AZ1512) followed by metal deposition of 5 nm-thick Ti and 50 nm-thick Au (AJA Ebeam Evaporator) and the liftoff process (rinsing samples in 65 °C acetone).

Second, we work on the fabrication of the bottom chip. Photonic devices, MEMS structures, and markers are fabricated on an SOI chip, using standard electron-beam lithography (JOEL, JBX-6300FS; E-beam resist: ZEP 520A) followed by deep reactive-ion etching (DRIE, Oxford Plasmalab 100 ICP) and e-beam resist removal. Next, metal patterns, including electrodes and bonding pads, are fabricated on the bottom SOI chip using standard optical lithography (LaserWriter, LW405b; photoresist: AZ1512) followed by metal deposition of 5 nm-thick Cr and 50 nm-thick Au (Lesker NANO 36 thermal evaporator) and the liftoff process (rinsing samples in 65 °C acetone). Then, we use the diluted hydrogen fluoride (DHF) for the release of MEMS structures. The 49% HF liquid is diluted with DI water in the ratio of 1:4. After 1.5 h of DHF release, the SOI chip is rinsed with acetone for 0.5 h and then dried using a critical point dryer (Leica EM CPD300). Next, we use the wire bonder (F&K Delvotec 5330) to place the aluminum solders on the bonding pads on both chips. Finally, these two chips are aligned and bonded together using the flip-chip bonder (FINEPLACER sigma) by thermal compression.

**Experimental Setup.** We use a quantum cascaded laser (Daylight, MIRcat-1200) covering the wavelength range from 3650 nm to 4150 nm. An optical chopper (Stanford Research SR540) is placed at the laser output. A half-wave plate (Thorlabs WPLQ5SM-4000) is placed right after the chopper to control the polarization. The light is focused on a ZnF₂ fiber end using a ZnSe lens to couple the MIR light from the tunable laser into the MIR fiber. The light is then coupled in and out of the PIC chip through two on-chip grating couplers. Both fiber ends are mounted on mechanical precision positioners with a 10° tilting from the vertical direction. An optical microscope is used to facilitate the fiber-to-chip alignment. Optical signals from the chip are detected with an MIR photodetector (Thorlabs PDA20H). The photodetector is connected to a lock-in amplifier (Stanford Research SR830) as the input signal. Meanwhile, the optical chopper is also connected to the lock-in amplifier as the reference signal to reduce the measurement noise. The Si-McS chip is electrically connected to a customized PCB via wire bonding. We use a semiconductor characterization system (Keithley 4200-SCS) for bias voltage supply to implement the time-domain modulation of OPD.

### ASSOCIATED CONTENT

#### Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acsphotonics.2c00381.

Waveguide design parameters and loss study; simulation details; experimental voltage calibration for the electrostatic actuation; estimation of the theoretical performance; validation of the linear superposition assumption; spectrum reconstruction robustness to measurement noise; testing setup and measured results for gas absorption spectroscopy; and comparison tables (PDF)

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Funding
We acknowledge Singapore Ministry of Education (MOE2019-T2-2-104) for financial support.

Notes
The authors declare no competing financial interest.

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