

Full length article

MHz-rate scanned-wavelength direct absorption spectroscopy using a distributed feedback diode laser at 2.3 μm

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HIGHLIGHTS

- MHz-rate scanned-wavelength TDLAS was demonstrated using a DFB laser.
- Excellent agreement was observed between direct absorption measurements and simulations.
- Tuning characteristics of DFB laser were examined up to a scan rate of 2 MHz.

ARTICLE INFO

Keywords:

Tunable diode laser absorption spectroscopy
Direct absorption spectroscopy
MHz scan rate
Distributed feedback laser

ABSTRACT

This paper demonstrates scanned-wavelength tunable diode laser absorption spectroscopy (TDLAS) with a scan rate up to 2 MHz using a distributed feedback (DFB) diode laser. The 2.3- μm DFB laser was used to probe the R (11) line present in the first overtone band of carbon monoxide (CO). Detailed tuning characteristics of the DFB laser were investigated over a wide range of scan rates from 20 kHz to 2 MHz. The tuning range was found to decrease exponentially with the scan rate below 1 MHz, and then slightly decrease up to 2 MHz. By applying a sinusoidal waveform to the injection current, the phase shift (ϕ) between intensity and frequency modulations was measured to be 1.11π at the scan rate of 20 kHz, which increases to 1.61π at 2 MHz. Due to the significant variation of ϕ with the scan rate, the position of the target absorption profile on the transmitted laser intensity curve must be adjusted accordingly based on the simultaneously recorded etalon signal. All the measurements obtained at different scan rates show excellent consistency in the CO spectrum. This study reveals that MHz-rate scanned-wavelength direct absorption spectroscopy can be developed for ultrafast gas sensing that may find promising applications in many fields.

1. Introduction

Tunable diode laser absorption spectroscopy (TDLAS) is a promising technique for the development of advanced sensors which can offer high sensitivity, high accuracy, high selectivity, and fast responsivity [1,2]. TDLAS-based gas sensors have been widely utilized for industrial process monitoring, combustion diagnostics, and greenhouse gas sensing [3–5]. This technique can be mainly categorized into two types, direct absorption spectroscopy (DAS) and wavelength modulation spectroscopy (WMS). Although WMS grasps more attention due to its effective noise rejection capability and improved robustness, DAS has still an invincible position in various conditions owing to its wide

applicability, relatively easy data interpretation, and simple implementation. Furthermore, its ability to direct absorbance profile measurements is uniquely beneficial specifically in determining the spectroscopic parameters [6]. A great number of studies have reported the application of TDLAS sensors for non-intrusive measurements of species concentration, pressure, and flow velocity [7–11].

In DAS with tunable diode lasers, the laser frequency is normally scanned across the target absorption line by tuning the injection current at the scan rate of Hz or kHz for temperature and species concentration measurements in many applications such as gas-turbine combustors, detonation engines, and scram-jets [12–14]. However, there is a pressing need to develop MHz-rate absorption sensor which can capture

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<https://doi.org/10.1016/j.optlastec.2020.106344>

Received 30 January 2020; Received in revised form 30 March 2020; Accepted 9 May 2020

Available online 22 May 2020

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the highly transient combustion processes in hybrid rockets and supersonic combustion systems in the time scale of microseconds [11]. Furthermore, MHz-rate diagnostic tools are also required to study the transient phenomenon in shock wave interaction processes [2]. It is well-known that the laser scan rate is linked with the response time of TDLAS measurements. Thus, it is important to investigate whether reliable spectroscopic measurements can be maintained when diode lasers are scanned at the MHz-rate.

Carbon monoxide (CO) is a major pollutant produced in incomplete combustion activities. It has rovibrational absorption bands at 1.55 μm , 2.3 μm and 4.6 μm that can be accessed by commercially available semiconductor lasers. The overtone and combination bands of CO at 1.55 μm could be exploited by the low-cost telecommunication diode lasers [15,16]. However, the detection sensitivity is limited due to the weak absorption strength at the near-infrared. Mid-infrared quantum cascade lasers or interband cascade lasers have been utilized to develop sensitive CO sensors [17,18], but these semiconductor lasers are still of limited use for practical applications due to their high cost. Therefore, low-cost distributed feedback (DFB) diode lasers are mostly used to exploit strong absorption lines of CO present at 2.3 μm . Chao *et al.* [19] demonstrated the CO sensing in the controlled laboratory environments of heated cell and a combustion exhaust rig by exploiting two absorption lines, R(10) and R(11) present in the first overtone band near 2.3 μm using a DFB diode laser. They also exploited the same CO sensor for *in situ* and real-time monitoring in a pulverized-coal-fired power plant [20]. However, no research has been reported on the development of MHz-rate absorption spectroscopy of CO using such a DFB laser.

In fact, the development of MHz-rate scanned wavelength DAS has been scarcely reported. Lackner *et al.* [21] performed the pioneering study of using a vertical-cavity surface-emitting laser (VCSEL) to probe the rovibrational transitions of methane (CH_4) at 1.68 μm in a static gas cell with scan rates up to 5 MHz. The scanned-wavelength DAS was used for high-speed absorption measurements. The tuning characteristics of VCSEL were also analyzed at 25 kHz to 1 MHz modulation frequencies when the laser was ramped with triangular waveforms. Kaebe *et al.* [22] demonstrated direct absorption temperature measurements in a shock tube also using a VCSEL with the highest modulation frequency of 800 kHz. The temperature was determined by scanning the VCSEL over the selected transitions (1391.67 nm, 1392.19 nm, 1392.33 nm, and 1392.53 nm) and using a variant method of two-line thermometry. The results were compared to the calculated temperatures and found to be in agreement within a single-scan standard deviation of ± 33 K. It can be inferred from the above literature review that only VCSELs have been implemented to realize MHz-rate scanned-wavelength DAS. Although VCSELs in the visible to near-infrared range are relatively mature devices, the application-grade room-temperature continuous-wave VCSELs beyond 2 μm are relatively less mature and less commercially available in the market [23,24]. Hence, the potential of using more widely used DFB semiconductor lasers for high-speed (MHz rate) scanned-wavelength DAS is valuable to be explored.

In this paper, ultra-fast 2 MHz scan-rate TDLAS is demonstrated based on the scanned-wavelength DAS with a DFB diode laser. Carbon monoxide (CO) was chosen as the target species for the validation of the ultrafast TDLAS. A DFB laser was utilized to exploit the absorption line R(11) of CO at 2.3 μm . The rapid tuning characteristics of the 2.3- μm DFB laser were comprehensively examined. The absorption measurements of CO were performed in a static gas cell at different scan rates (20 kHz – 2 MHz) to illustrate the accuracy and precision.

2. Methodology

A detailed theoretical explanation of absorption spectroscopy has been well documented elsewhere [25]. Here, only a brief description of scanned-wavelength DAS is presented and subsequently used in this

work. Absorption spectroscopy is based on the Beer-Lambert law, which relates the incident laser intensity (I_0) and transmitted laser intensity (I_t) through a uniform gas medium as:

$$(I_t/I_0)_\nu = \exp(-\alpha_\nu) = \exp(-S(T)Px_{\text{abs}}\phi_\nu L) \quad (1)$$

where α_ν denotes the spectral absorbance at frequency ν , $S(T)$ ($\text{cm}^{-2} \text{atm}^{-1}$) is the line-strength of a specific transition which changes only with temperature, P (atm) is the total pressure of the absorbing species, x_{abs} represents the species mole fraction, ϕ_ν is the line-shape function, and L (cm) is the absorption path length.

Scanned-wavelength DAS targets one or a group of transitions of interest by tuning the laser wavelength. By using Beer-Lambert law shown in Eq. (1) and tracking the wavelength variation in time with an etalon, one can infer the absorbance as a function of wavelength. An integrated absorbance area (A) of a particular transition can be acquired by using the Voigt fitting of the absorbance profile:

$$A = \int_{-\infty}^{\infty} a_\nu d\nu = Px_{\text{abs}}S(T)L \int_{-\infty}^{\infty} \phi_\nu d\nu = Px_{\text{abs}}S(T)L \quad (2)$$

With the knowledge of the absorption path length (L) and total gas pressure (P), the species mole fraction (x_{abs}) can be determined accordingly.

In scanned-wavelength DAS, the requirement of precise knowledge of the absolute wavelength is eased as long as the scan range covers the whole portion of the target transition. This extensively decreases the complexity and price of a practical sensor especially when it is applied for field applications. Additionally, since the line-shape function is normalized to 1 in Eq. (2), the parameters such as broadening coefficients and their relevant temperature dependence are not required to be known. This effectively reduces the workload for sensor validation and uncertainty in approximating the species composition.

3. Experimental setup

The experimental setup of high-speed detection of carbon monoxide (CO) is shown in Fig. 1. A continuous-wave (CW) DFB laser (Nanoplus, Germany) at 2.3 μm was used to exploit the R(11) transition of CO centered at 4300.7 cm^{-1} . This particular CO absorption line has been used for CO measurements in the laboratory-scale combustion test rig, heated static gas cell and pulverized coal-fired power plant [20,26,27]. Temperature and injection current of the DFB laser were controlled by a chassis mount temperature controller and a current controller (Wavelength Electronics, Inc.), respectively. A function generator (Rigol DG 4162, out impedance 50Ω) was used to control the laser modulation current. In this work, the DFB laser was sinusoidally modulated across the target absorption line by feeding waveforms with modulation frequency (10 kHz – 1 MHz) to the current controller, thus enabling the measurement scan rate of 20 kHz to 2 MHz (two laser scans per modulation cycle). A germanium (Ge) etalon with a free spectral range (FSR) of 0.0164 cm^{-1} was employed to track the relative frequency response when scanning the laser injection current.

The target absorption line of CO was recorded at the pressure of 30 torr in a static gas cell. The gas pressure was monitored using a pressure meter (Bronkhorst, Inc) with an accuracy of $\pm 0.5\%$ up to 1350 torr. The laser beam was directed through the gas cell (absorption path length, $L = 40 \text{ cm}$) filled with 0.94% CO/N_2 and then the transmitted laser beam was focused on the infrared photodetector (Vigo Ltd.) with a gold-coated concave mirror (focal length, 50 mm).

All the experimental data were acquired by a Tektronix MDO3014 mixed domain oscilloscope with 100 MHz bandwidth and 2.5 GS/s sampling rate. Before each absorption measurement, the incident laser intensity (I_0), also known as the baseline, was measured first by purging the gas cell. It should be noted that the determination of such a baseline is one of the major uncertainty sources for scanned-wavelength DAS.

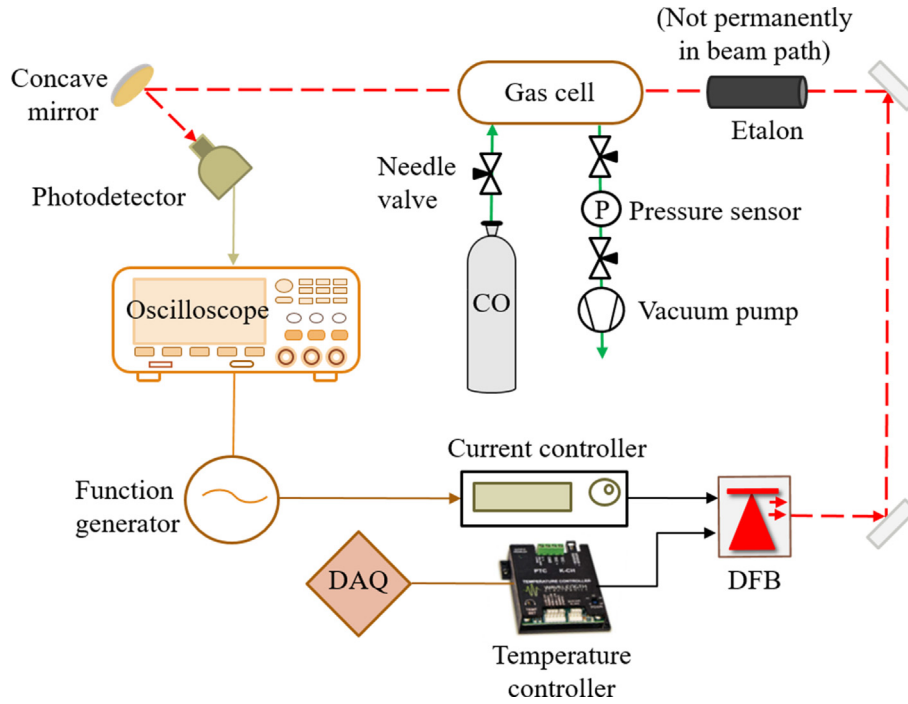


Fig. 1. Experimental setup of the scanned-wavelength direct absorption spectroscopy.

4. Results and discussion

4.1. Characterization of 2.3 μm DFB diode laser

Besides the advantages of low-noise operation, single-mode stability, and narrow linewidth [28], the DFB diode laser offers rapid tuning characteristics that are beneficial to achieve effective time resolution when noise is insignificant during TDLAS measurements. Here, the tuning characteristics of the DFB laser were first comprehensively examined. The variation of DFB laser power and frequency with the injection current was characterized using a spectral analyzer (Bristol Instruments, accuracy ± 0.75 ppm) and a power meter (Ophir Optronics). Fig. 2(a) shows the laser tuning characteristics as a function of injection current at various temperatures (24 $^{\circ}\text{C}$ – 32 $^{\circ}\text{C}$). The measured laser power varies from 2 mW to 5.4 mW over the tested temperature range at the maximum laser injection current of 110 mA. This DFB laser can be tuned over the range of 4294.40 cm^{-1} to 4303.30 cm^{-1} by varying the laser injection current and temperature. The target R(11) line of CO centered at 4300.7 cm^{-1} , shown as a brown color dashed line in Fig. 2(a), can be well covered by the 2.3 μm DFB laser. The laser power and frequency demonstrate a linear relationship with the injection current especially when the current is below 90 mA.

It is known that the modulation of the injection current of a diode laser at an angular frequency $\omega = 2\pi f$ produces both modulations of frequency and intensity [29]:

$$v(t) = \bar{v} + a \cos(\omega t) \quad (3)$$

$$I_0(t) = \bar{I}_0 [1 + i_0 \cos(\omega t + \phi)] \quad (4)$$

where \bar{v} (cm^{-1}) is the center laser frequency, a (cm^{-1}) is the modulation depth, i_0 is the linear intensity amplitude normalized by the average laser intensity \bar{I}_0 , and ϕ is the linear phase shift between intensity and frequency modulations (IM-FM phase shift).

In order to investigate the phase shift ϕ , the injection current of the DFB laser was ramped sinusoidally at different scan rates. Fig. 2(b) depicts the measured laser transmission and etalon signals of the DFB laser at 1-MHz rate. The wavelength turning points define the minimum and the maximum of the wavelength modulation. Note that the

modulation amplitude was fixed at 20 mA for all the measurements. The spectral distance between two adjacent fringes on the etalon signal is considered as one FSR (0.0164 cm^{-1}). The frequency response of the DFB laser is demonstrated by the sinusoidal fitting with a frequency modulation depth of 0.09 cm^{-1} shown in Fig. 2(b); here the modulation depth is defined as half of the peak-to-peak value.

It has been reported that the phase shift between intensity modulation and frequency modulation (IM-FM phase shift ϕ) is not a certain π value, which varies with the scan rate [29,30]. Fig. 3 shows the variation of IM-FM phase shift with the scan rate of laser injection current from 20 kHz to 2 MHz. The increasing trend of ϕ was observed with the increased scan rate, i.e., 1.11π at 20 kHz to 1.61π at 2 MHz. Such a phase shift dependence can be linked to the complex thermal behavior of the DFB laser under the modulation of injection current.

Fig. 4 illustrates the tuning range of the DFB laser as a function of scan rate (20 kHz to 2 MHz) at four different amplitudes of modulation currents. It is observed that the tuning range decreases with an increased scan rate. For the case of 85 mA amplitude of modulation current, the tuning range exponentially decreases at the rate of 0.19 $\text{cm}^{-1}/100$ kHz between 20 kHz and 1 MHz. However, it experiences nearly a linear decrease of 0.02 $\text{cm}^{-1}/100$ kHz between 1 MHz and 2 MHz. In case of small amplitude modulation currents, particularly at 20 mA, the tuning range also reduces as shown in Fig. 4 but with a lower rate. This could mainly be attributed to the thermally-induced frequency tuning which is a slow effect and linked to the thermal properties of diode lasers [30].

4.2. CO absorption measurement

The temporal resolution of scanned-wavelength DAS governed by the scan rate is inferior because of the large bandwidth demand of sawtooth or triangular waveform on the detection system. Therefore, the sinewave modulation is applied for high-speed absorbance measurements.

The R(11) line of 0.94% CO was measured at different scan rates such as 20 kHz, 200 kHz, and 2 MHz in this work. First of all, Fig. 5 shows the CO absorption measurement at 20 kHz scan rate and 30 torr pressure. A sinusoidal waveform with an amplitude of 20 mA was used

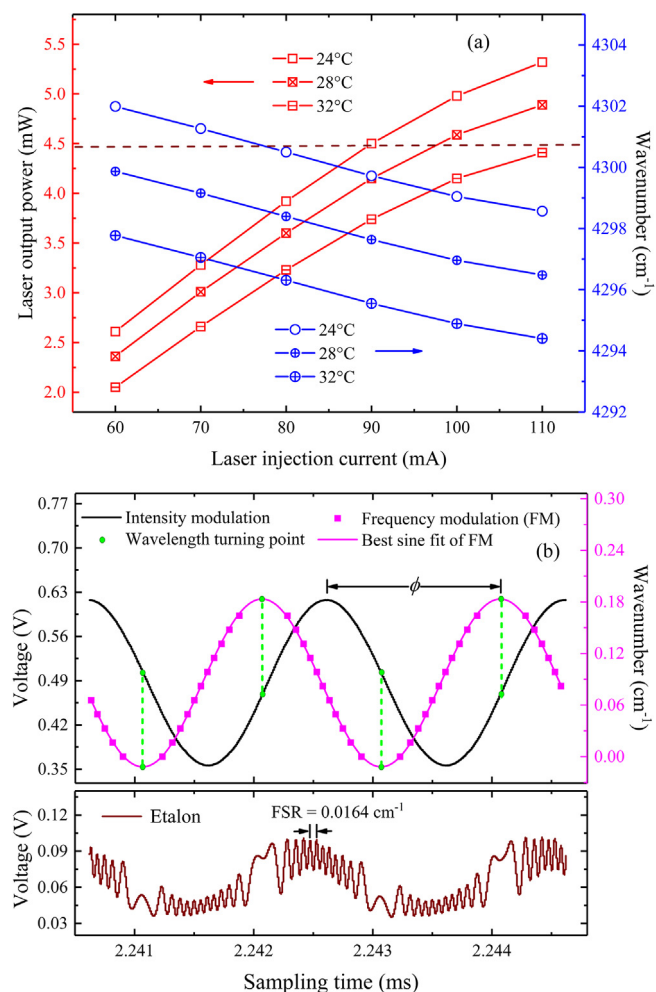


Fig. 2. (a) Variation of laser output power (mW) and frequency (cm^{-1}) with laser injection current (mA) at different laser temperatures. (b) Laser intensity and frequency modulation measurements at 1-MHz scan rate of the injection current.

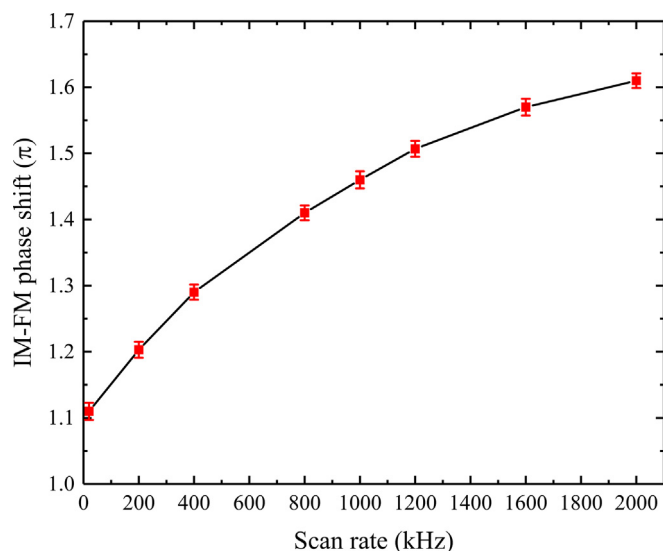


Fig. 3. Variation of the IM-FM phase shift with the scan rate of laser injection current from 20 kHz to 2 MHz.

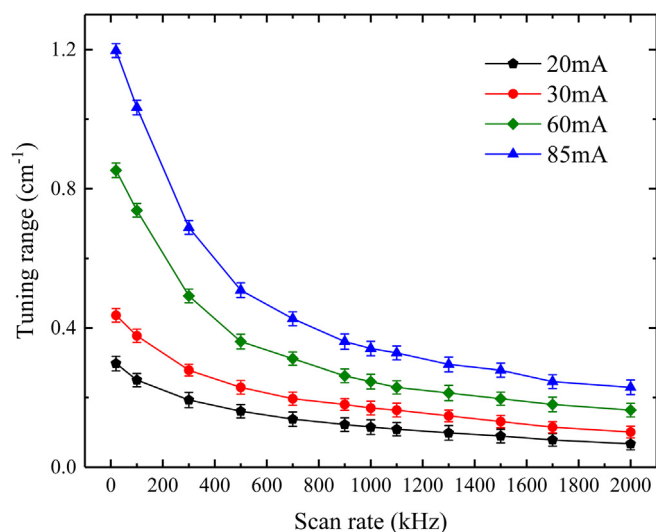


Fig. 4. Variation of the tuning range of the DFB laser with the scan rate at four different amplitudes of modulation currents (20 mA, 30 mA, 60 mA, and 85 mA).

to scan the laser wavelength across the target absorption line. The fitted baseline (I_0) and transmitted laser intensity (I_t) signals for a single scan are depicted in Fig. 5(a). The resultant absorbance fitted with the Voigt profile is illustrated in Fig. 5(b); and the fitting residual ($\pm 4\%$) is plotted at the bottom panel of Fig. 5(b). Similarly, the representative absorption measurement of CO at 200 kHz and the pressure of 30 torr is depicted in the Supplementary Fig. S1. By comparing the measured absorption profiles at 20 kHz and 200 kHz, it is observed that both measurements are almost identical regarding the line broadening ($\sim 4.5\%$ deviation in the full width at half maximum) and absorption peak value (0.8% deviation).

In comparison, the high-speed CO absorption measurement at the scan rate of 2 MHz is depicted in Fig. 6. The baseline (I_0), transmission signal (I_t), and etalon signal measured at 2 MHz are shown in Fig. 6(a). There exists a phase shift of 1.61π between the intensity and frequency modulations for this particular DFB laser. Therefore, the position of CO absorption, as shown in Fig. 6(a), was adjusted near the crest or trough of the sinusoidally modulated I_t curve according to the recorded etalon signal. It should be noted that fitting the non-absorption region of I_t curve is important in determining the accurate absorption profile. A MATLAB program was designed to efficiently fit the non-absorption region. Fig. 6(b) compares the two measured CO absorbance profiles, corresponding to the falling (V_1V_2) and rising (V_2V_3) in Fig. 6(a), along with the best-fitted Voigt line-shape curves. The CO absorbance profiles agree well with the Voigt fitting curves, yielding a residual within $\pm 3\%$ shown at the bottom panel of Fig. 6(b). The two absorption measurements within a modulation cycle are in excellent agreement with each other.

Finally, all the absorption measurements at different scan rates (20 kHz, 200 kHz, and 2 MHz) are compared with the HITRAN simulation and found to be in good agreement as shown in Fig. 7. It is worthy of note that the bandwidths of photodetector, oscilloscope or DAQ card are the critical parameters that may affect the measurement accuracy. As reported in [21], a vivid instrument broadening can occur when the bandwidth of the detection system does not match with the scan rate. Thus, a photodetector with sufficiently high bandwidth must be used to achieve high-speed accurate absorbance measurements. Considering the above-discussed viewpoints, we employed 2.5 GS/s sampling rate oscilloscope and 10-MHz bandwidth photodetector which were found to be sufficient for fast response (2 MHz) CO absorption measurements.

In this work, the uncertainties of TDLAS measurements at different

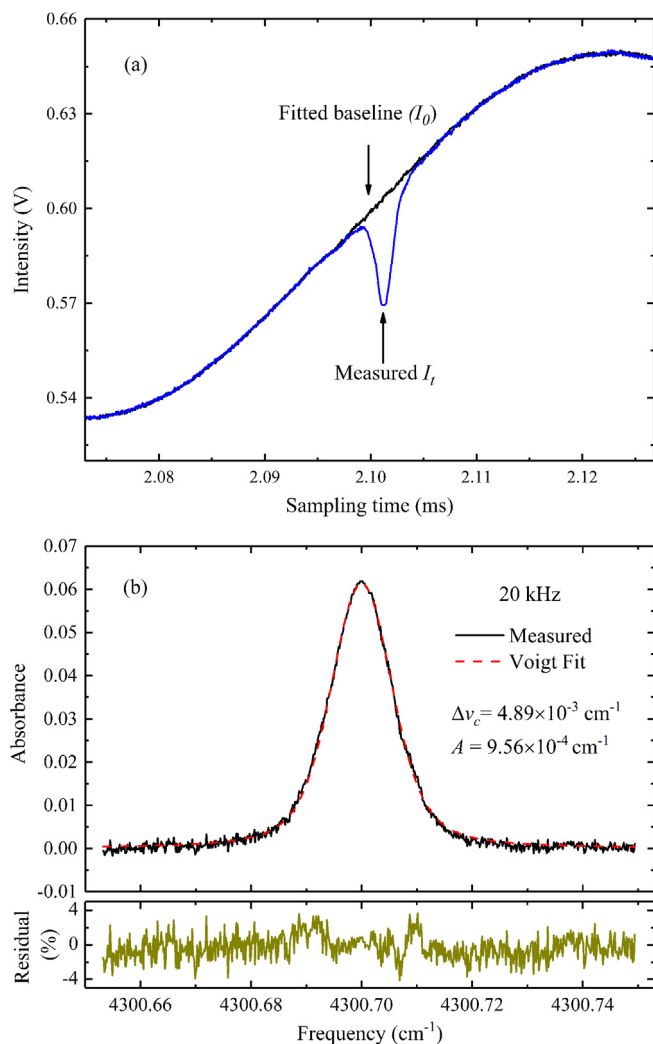


Fig. 5. (a) Laser baseline (I_0) and transmission (I_i) signal of the CO absorption measurement at 30 torr with a 20-kHz sinusoidal scan. (b) Measured CO absorbance with the Voigt fitting and fitting parameters including collisional width (Δv_c) and integrated area (A) (top panel) alongside the corresponding residual (bottom panel).

scan rates were estimated to be 1.3% for 20 kHz, 1.0% for 200 kHz, and 1.3% for 2 MHz by mainly taking into account the line-strength uncertainty and Voigt-fitting error. With the current optical setup, a signal-to-noise (SNR) of 72, 75, and 92 was obtained for 0.94% CO and 40-cm path length at the scan rate of 20 kHz, 200 kHz, and 2 MHz, respectively. Hence, we achieved a minimum detection limit (MDL) of 130 ppm CO at 20 kHz, 124 ppm at 200 kHz, and 103 ppm at 2 MHz, respectively. It is of interest to observe that the MDL at the MHz scan-rate is improved by $\sim 20\%$ compared to that at the kHz-rate. The detailed investigation discloses the capability of the developed ultra-fast DFB-based TDLAS to measure CO absorption at MHz scan rate using scanned-wavelength DAS. The developed MHz-rate TDLAS has a promising potential to be used in combustion and propulsion environments to examine transient phenomena due to its superior time response.

5. Conclusions

The development of MHz-rate TDLAS was demonstrated by exploiting the R(11) line of CO using scanned-wavelength DAS. The tuning range of the 2.3- μm DFB laser was also examined at different scan rates (20 kHz–2 MHz) and currents (30–85 mA). When the DFB laser was ramped as a symmetric triangle with 85 mA amplitude, a

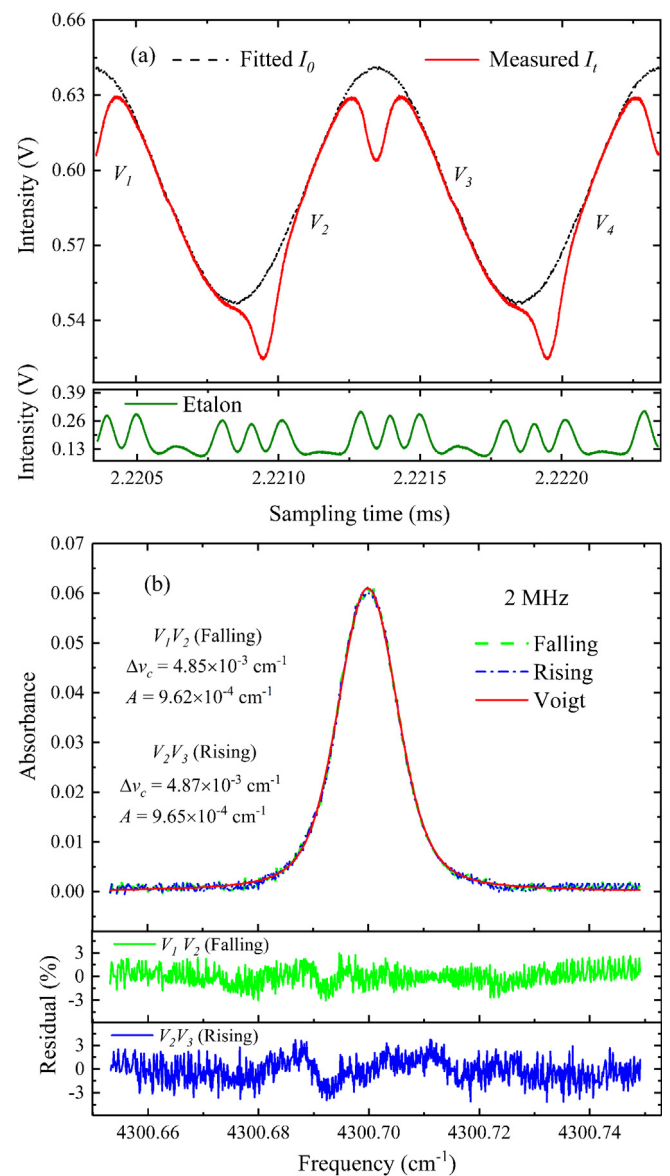


Fig. 6. (a) Laser baseline (I_0) and transmission signal (I_i) of the CO absorption measurement at 30 torr with 2-MHz sinusoidal scan rate and 20-mA modulation amplitude. (b) Measured CO absorbance, falling (V_1V_2) and rising (V_2V_3), with the Voigt fitting and fitting parameters including collisional width (Δv_c) and integrated area (A) (top panel) alongside the corresponding residual (bottom panel).

decreasing trend of the tuning range ($0.19 \text{ cm}^{-1}/100 \text{ kHz}$) was observed with the increasing scan rate from 20 kHz to 1 MHz but the tuning range reduces slightly ($0.02 \text{ cm}^{-1}/100 \text{ kHz}$) as the scan rate increases from 1 MHz to 2 MHz. The MHz-rate TDLAS was then demonstrated by modulating the DFB laser sinusoidally with a 20 mA modulation amplitude to scan the laser wavelength over the target absorption line. The typical absorption spectrum of the R(11) of CO was measured at 30 torr using different scan rates of 20 kHz, 200 kHz, and 2 MHz. It was found that all the measurements at different scan rates were in good agreement with each other and the HITRAN simulation. This study presents the initial demonstration of ultra-fast response (μs) scanned-wavelength DAS that will find more applications in combustion diagnostics.

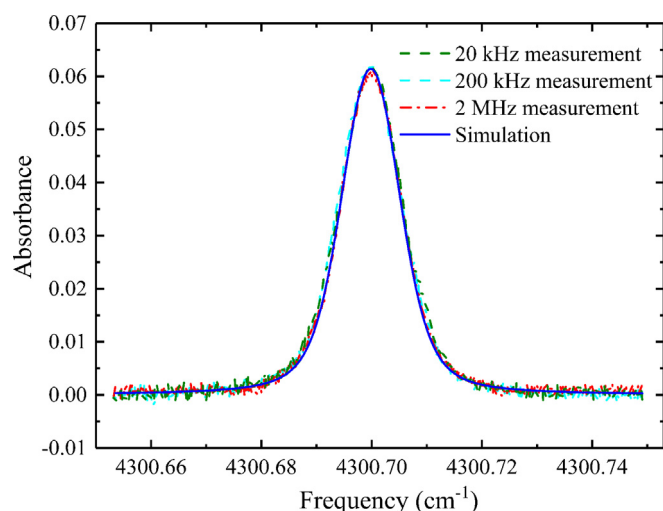


Fig. 7. Comparison of CO absorption measurements at different scan rates of 20 kHz, 200 kHz, and 2 MHz with HITRAN simulation (0.94% CO/N₂, T = 23 °C, P = 30 torr, and L = 40 cm).

CRedit authorship contribution statement

Mohsin Raza: Conceptualization, Methodology, Investigation, Formal analysis, Validation, Visualization, Writing - original draft, Writing - review & editing, Conceptualization, Methodology, Investigation, Formal analysis, Validation, Visualization, Writing - original draft, Writing - review & editing. **Liuha Ma:** Methodology, Investigation, Supervision. **Chenyu Yao:** Methodology, Investigation. **Min Yang:** Methodology, Investigation. **Zhen Wang:** Methodology, Investigation. **Qiang Wang:** Methodology, Supervision. **Ruifeng Kan:** Methodology, Supervision. **Wei Ren:** Conceptualization, Methodology, Formal analysis, Validation, Visualization, Writing - review & editing, Supervision, Project administration, Funding acquisition.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

This work is supported by National Natural Science Foundation of China (51776179), Research Grants Council of the Hong Kong SAR, China (14234116), and Open Research Fund from the State Key Laboratory of Applied Optics (SKLAO-201901).

Appendix A. Supplementary material

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.optlastec.2020.106344>.

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