Photonic MEMS for NIR in-situ Gas Detection and Identification

Tiziana C. Bond, Garrett D. Cole, Lynford L. Goddard, and Elaine M. Behymer
Meso, Micro, Nano Technology Center
Lawrence Livermore National Laboratory
Livermore, CA 94550, USA
bond7@llnl.gov

Abstract—We report on a novel sensing technique combining photonics and microelectromechanical systems (MEMS) for the detection and monitoring of gas emissions in environmental, medical, and industrial applications. We discuss how MEMS-tunable vertical-cavity surface-emitting lasers (VCSELs) can be exploited for in-situ detection and NIR spectroscopy of several gases, such as O2, N2O, CH4, HF, HCl, etc., with estimated sensitivities between 0.1 and 20 ppm on footprints << 10^-3 mm^3. The VCSELs can be electrostatically tuned with a continuous wavelength shift up to 20 nm, allowing for unambiguous NIR signature determination. Selective concentration analysis in heterogeneous gas compositions is enabled, thus paving the way to an integrated optical platform for multiplexed gas identification by bandgap and device engineering. We will discuss here, in particular, our efforts on the development of a 760 nm AlGaAs-based tunable VCSEL for O2 detection.

I. INTRODUCTION

Gas analysis is typically carried out using laboratory analytical techniques, i.e. gas chromatography or mass spectrometry (GC-MS), which do not satisfy current device and material constraints for unattended, flexible ground sensors, or for lightweight, highly sensitive systems for avionic operations. IR absorption spectroscopy is the current alternative powerful approach for in-field detection and identification, and several interesting techniques have been developed including tunable diode laser absorption spectroscopy (TDLAS) [1]. Recently, MEMS tunable VCSELs have been implemented in such fashion for NIR spectroscopy [2]. Unfortunately, many existing TDLAS systems exhibit drawbacks that limit their deployment including the need for cryogenic cooling and a requirement for either bulky multipass cells, or long hollow or porous fiber, with a relatively slow time response [3]. We herein present the extension of TDLAS to a miniaturized gas in-situ detection system utilizing MEMS-tunable optoelectronic devices.

This technology relies on extended coupled cavity (ECC) MEMS-tunable VCSELs [4] in which the epitaxial materials structure is engineered to align the laser emission to a specific absorption wavelength (coarse tuning); additionally, these devices incorporate a micromechanically tunable optical cavity that allows for scanning of the emission wavelength over a wide and continuous range, allowing access to multiple absorption lines of the gas (fine tuning). In addition, when gases without a significant NIR signature are to be detected, complimentary techniques can be implemented on the same platform. Functionalizing the cavities with gas-sensitive coatings allows for enhanced detection through a change in the optical response of the coating (e.g. index shift, change in absorption, etc.). Resonant cavities with high quality factor (Q) amplify the magnitude of these changes. The details of this latter approach, particularly applied to H2 sensing in an edge-emitting laser structure, are described in [5]. Finally, techniques including cavity ring down spectroscopy (CRDS) can be implemented to increase the sensitivity [6].

Figure 1. Cross-sectional schematic of the MEMS tunable ECC-VCSEL for O2 sensing. The presence of gas in the air gap quenches the laser emission when the resonance wavelength is tuned to correspond with an appropriate absorption line.

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II. DEVICE DESIGN

The operation of the tunable-VCSEL-based gas sensor can be described as a multipass cell with optical gain. A sketch of this device is shown in Fig. 1. In operation, the laser is electrically driven above threshold; the gas flowing through the air gap spoils the gain-loss balance necessary for lasing by increasing the absorption losses within the cavity. In this case the high-Q of the VCSEL structure enhances absorption as the light is reflected several (>100) times within the resonant cavity, between the top and bottom distributed Bragg reflectors (DBRs). During operation, the lasing power can be monitored remotely via transmission through an optical fiber or directly via an integrated detector.

A. Tuning Range and Sensitivity

In order to efficiently and selectively detect the signature absorption lines of the gas of interest, it is critical to design an appropriate tunable optical cavity. The absorption cross-section of O$_2$ around 760 nm is shown in Fig. 2 (a). For our tunable VCSEL we desire the laser linewidth ($\delta\lambda$) to be < 1 pm within a full scanning range of at least 10 nm, an actuation voltage of < 10 V, and a power consumption on the order of tens of mWs. In Fig. 2 (b) the threshold gain vs. wavelength is calculated showing the capability of continuous tuning over 20 nm within the wavelength range of interest. Dynamic mode-hop free tuning is inherent in MEMS-tunable VCSELs due to the extremely short axial cavity length. Thus, the wavelength resolution of the tunable laser is limited by the voltage source driving the electrostatic actuator, the stability of the micromechanical system, as well as the resolution of the read-out system.

![Graph](image1)

The presence of gases in the VCSEL air gap affects the amplification factor or round trip enhancement of the power flow in the laser structure and thus the variation of output power when compared with the quiescent state $P_0$:

$$\frac{\Delta P}{P} = \frac{P_o - P}{P_o} = \frac{A_0 - A}{A_o}.$$  \hspace{1cm} (1)

The amplification factor in absence of any gas is given by:

$$A_0 = (1 - \exp(-\delta\lambda L_{\text{Cavity}}))^{-1}$$  \hspace{1cm} (2)

where $\delta\lambda = \alpha_0 - \Gamma g$ is the margin between the losses and the net modal gain of the laser weighted by the modal overlap $\Gamma$. Similar to the Beer-Lambert law, the absorption of the chemical species is accounted in $A$ through the relative gas cross-section $\sigma_{\text{gas}}$:

$$\alpha_\text{gas} \left( \text{cm}^{-1} \right) = \sigma_{\text{gas}} C.$$  \hspace{1cm} (3)

where $C$ is the volume concentration of the gas species. In such case $\delta\lambda$ becomes equal to $\alpha - \alpha_{\text{gas}} - \Gamma g$.

The limit of detection (LOD) of the sensor platform is determined by a combination of the device and measuring system sensitivity. In our initial evaluation we have taken into account the system resolution by considering a conservative instrumentation limit of $\Delta P/P = 10^{-3}$. An analytical analysis of the sensitivity of our lasers shows that for O$_2$ with a cross-section $\sigma_{\text{NIR}} \approx 4 \times 10^{-22}$ cm$^2$/molecule, at the operation wavelength of 760 nm for a bias current twice the threshold value, an LOD $\approx 20$ ppm of volume in air can be obtained in a 50 $\mu$m diameter VCSEL with an air-gap thickness $L = 5$ $\mu$m. If we extend the analysis to other gases with similar or higher NIR cross-sections the LOD is very promising showing sensitivities to few ppm, (TABLE I. . For thicker air-gaps the sensitivity would increase as shown in Fig.3. Cross-sections were derived from MUITRAN database assuming (assuming a broadening factor ~0.01cm$^{-1}$)

<table>
<thead>
<tr>
<th>Gas</th>
<th>$\lambda$ (m)</th>
<th>$\sigma$ (cm$^2$/mol)</th>
<th>LOD</th>
</tr>
</thead>
<tbody>
<tr>
<td>O$_2$</td>
<td>0.76</td>
<td>$10^{-21}$</td>
<td>20 ppm</td>
</tr>
<tr>
<td>HF</td>
<td>1.27</td>
<td>$10^{-19}$</td>
<td>0.1 ppm</td>
</tr>
<tr>
<td>N$_2$O</td>
<td>1.38</td>
<td>$10^{-21}$</td>
<td>10 ppm</td>
</tr>
<tr>
<td>CH$_4$</td>
<td>1.65</td>
<td>$10^{-20}$</td>
<td>1 ppm</td>
</tr>
<tr>
<td>HCl</td>
<td>1.75</td>
<td>$10^{-19}$</td>
<td>0.1 ppm</td>
</tr>
</tbody>
</table>

Figure 2. (a) Signature of O$_2$ at ~760-HITRAN source; (b) modeled laser threshold gain displaying continuous emission tuning for O$_2$ sensing.
B. Design and Fabrication of ECC VCSEL for O₂ sensing

Oxygen sensors are very important in controlling automotive and industrial emission processes for lower pollution and better yields, as well as improving flight safety. Concentration monitoring is also very important for biosensors in clinical diagnosis. These and fabrication motivations have induced us to focus our development efforts on tunable VCSELs optimized for O₂ sensors.

For the tunable VCSEL, the suspended mirror structure is built atop a 760 nm AlGaAs “half-VCSEL” with a design similar to that outlined in [9]. A cross-sectional schematic of the tunable VCSEL is presented in Fig. 1. The AlGaAs epitaxial structure consists of a 40.5 period bottom DBR—

with linear composition grading between the high index (Alₐ₀.₃₀Ga₀.₇₀As) and low index (Alₐ₀.₉₂Ga₀.₀₈As) layers—and an active region incorporating three 8-nm Alₐ₀.₁₄Ga₀.₈₆As quantum wells (QWs) separated by 10-nm thick Alₐ₀.₄₀Ga₀.₆₀As barriers (band diagram depicted in Fig. 5). The peak gain of the active region is designed to be near the absorption maxima of molecular O₂ in this wavelength range, as shown in Fig. 2. Due to the strong absorption of the GaAs substrate, the VCSEL is constrained to be top-emitting, in this case through the MEMS-tunable mirror structure. Ohmic contacts to the VCSEL are provided by a Ti/Pt/Au p-contact annulus and a blanket deposited Ge/Au/Ni/Au contact on the backside of the n-doped substrate. Carrier and optical confinement are realized by non-selectively wet etching a shallow mesa and oxidizing an exposed Alₐ₀.₉₈Ga₀.₀₂As layer.

From the top down, the suspended mirror structure consists of an evaporated dielectric DBR (7 periods of TiO₂/SiO₂) on top of a tensile stressed (328 MPa) SiNx structural film deposited via plasma-enhanced chemical-vapor deposition (PECVD). The combination of the TiO₂/SiO₂ stack and nitride membrane forms a 7.5-period DBR including the SiNx layer as a high index quarter-wave layer. The tunable optical cavity utilizes the ECC design discussed in [4] and demonstrated most recently in [10]. In order to realize the extended cavity structure, a single film anti-reflection coating is included at the interface between the gain medium and air gap to eliminate coupled-cavity effects [11]. Including the large index discontinuity between the nitride membrane and air gap, the peak reflectivity of the top DBR is calculated to be 0.997.

For tuning of the emission wavelength, the device incorporates an integrated micromechanical actuator.
An applied bias across the aluminum contact on top of the SiN_{x} structural film and the p-contact on the VCSEL mesa creates an electrostatic force that displaces the suspended mirror towards the substrate, reducing the optical path length and blue-shifting the resonance wavelength. As mentioned previously, by the short cavity length of the VCSEL, wide and continuous single-mode tuning is possible in these devices. Previous demonstrations of electrically injected tunable VCSELS utilizing the ECC-design (emitting within the telecom relevant wavelength range near 1550 nm) have demonstrated tuning ranges approaching 70 nm [10]. For the devices presented here, the use of the integrated electrostatic actuator allows for a rapid tuning response. Characterization of this micro mechanical structure has demonstrated a near critically-damped response at atmosphere with a wavelength tuning time of < 10 μs [12]. As evident from Fig. 4 we have developed a viable process for the tunable mirror structure and are now focusing on fabricating and characterizing these structures on 760-nm VCSEL epi-material.

C. Future Direction

For gases lacking significant NIR signatures, such as H\textsubscript{2}, we can enhance the detection sensitivity by adding a gas-specific coating to the optical cavity. Here, it is critical to understand the appropriate coatings as well as their selectivity and specificity. Appropriate coatings include WO\textsubscript{3}, SnO\textsubscript{2}, PdO, ZnO, and porous Si, for use in monitoring NO\textsubscript{x}, CO, H\textsubscript{2}S, Cl\textsubscript{2} etc. These coatings will exhibit changes in refractive index when exposed to the appropriate target gas species, resulting in a measurable wavelength shift in the laser output spectrum. The basic technology outlined in this work is promising in that it can be extended to several material systems in the visible, as well as the short wavelength infra-red range (2-3 μm) where molecules have higher absorption cross-sections. Recent developments have led to the demonstration of micromechanically-tunable filter structures integrated with HgCdTe materials structures for widely tunable resonant detectors in this wavelength range [13]. Additionally, the technology has the potential of being extended to highly sensitive CDRS by integrating active (laser, detector) and passive devices (low loss filters) on the same platform [6].