

Quantum cascade laser spectrometer for trace-gas detection of exhaled Carbonyl Sulfide

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Abstract: Simultaneous concentration measurements of exhaled carbonyl sulfide and carbon dioxide were demonstrated using a pulsed quantum cascade laser based gas sensor. This sensor has potential applications in biomedical diagnostics such as in lung transplant rejection.

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Detection and analysis of carbonyl sulfide (COS) is of importance in a number of applications that include atmospheric chemistry and more recently in medical diagnostics. Elevated COS concentrations in exhaled breath have been reported in lung transplant recipients suffering from acute rejection [1] as well as patients with liver disease [2]. The low parts-per-billion (ppb) concentration range of many volatile molecular species in human breath presents technical challenges for clinical breath analysis applications, which require rapid, *in situ*, detection of trace-gases. However, in contrast to the currently used invasive diagnostic methods (e.g. bronchoscopic lung biopsies to assess lung transplant acute rejection), rapid analysis of expired breath using mid infrared laser absorption spectroscopy (MIRLAS) is a desirable non-invasive alternative. Application of a quantum-cascade (QC) laser in contrast to other mid-infrared sources allows the design of a compact, sensitive user-friendly, and liquid-nitrogen free trace-gas sensor suitable for potential medical diagnostics. In this work we report on the development of a MIRLAS gas sensor utilizing a quasi room temperature QC laser for simultaneous detection of COS and carbon dioxide (CO₂) in expired breath. The sensor architecture is similar to the one reported in Ref. 3 and 4. The thermoelectrically cooled QC laser operates in a pulsed mode at 4.85 μm and can be tuned between 2054.5 and 2060.5 cm^{-1} , which covers a number of strong absorption lines (line intensities $> 1 \times 10^{-18} \text{ cm}^{-1} / \text{molecule} \cdot \text{cm}^{-2}$) in the P branch of the COS fundamental rotational-vibrational spectrum. To minimize pulse-to-pulse fluctuations, the reference and sample beam signals are measured by means of a single photovoltaic HgCdTe detector followed by time resolved data acquisition electronics. The QC laser is driven by 25 ns current pulses with repetition rates up to 500 kHz, limited mainly by the data acquisition electronics. Wavelength scanning is performed using fast modulation of the laser sub-threshold current. Feedback electronics are applied for stabilization of laser power fluctuations resulting from the wavelength tuning process. This technique results in an improved signal-to-noise (S/N) ratio as well as stabilizing the laser linewidth. The absorption spectrum is digitized and recorded using a fast data acquisition card. To date, the noise equivalent sensitivity of the sensor for 1000 averaged frequency scans has been estimated to be ~ 3 ppb. A digital signal processing (DSP) platform for biogenic trace gas sensors is also in development to provide fast data acquisition (>1 MHz), standalone data processing functions, increased reliability, and enhanced sensor portability. As such, the sensor will be able to improve sensor data acquisition, while simultaneously satisfying space and safety constraints related to a medical setting.

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