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Spectroscopic Measurement of Air Temperature

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Abstract Optical dimensional measurements have to be corrected for the refractive index of air. The refractive index is conventionally calculated from parameters of ambient air using either Edlén or Ciddor equations or their modified versions. However, these equations require an accurate knowledge of ambient conditions and especially the temperature of air. For example, to reach an uncertainty of 10^{-7} in dimensions, the air temperature has to be known at $\sim$100 mK level. This does not necessarily cause problems in a stable laboratory environment. However, if measurements are done outdoors or in an industrial environment, variations in temperature can be very rapid and local temperature gradients can cause significant error if not taken into account. Moreover, if the required distance is long, the temperature over the whole measurement path can be impractical or impossible to determine at sufficient temporal or spatial resolution by conventional temperature measurement techniques. The developed method based on molecular spectroscopy of oxygen allows both lateral spatial and temporal overlap of the temperature measurement with the actual distance measurement. Temperature measurement using spectroscopy is based on a line intensity ratio measurement of two oxygen absorption lines, previously applied for measurements of high temperatures in flames. The oxygen absorption band at 762 nm is a convenient choice for two-line thermometry since the line strengths are practical for short- and long-distance measurements and suitable distributed feedback lasers are commercially available. Measurements done on a 67 m path at ambient conditions demonstrate that the RMS noise of 22 mK, or 7.5×10^{-5}, near 293 K using 60 s measurement time can be achieved, which is to our knowledge the best reported resolution.

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1 Introduction

Tunable diode-laser-based gas temperature sensors have been studied extensively during recent years [1–6]. Much of the research has been focused on combustion applications at elevated temperatures. Before room temperature semiconductor diode lasers were available, the laser sensors were based on impractical ring dye lasers and the measurements were performed in the UV range [1]. Nowadays semiconductor lasers provide robust and tunable light sources in the near-infrared (NIR) region and they are often used to probe absorption lines of oxygen or water that are common substances in combustion gases [2–6]. Especially in hot and rapidly changing combustion processes, optical techniques provide several benefits compared to more intrusive methods. Spectroscopic sensors offer fast response, excellent lateral spatial resolution, and overlap with minimal perturbation to the existing system. Acoustic thermometry has similar benefits as laser-based devices, but it cannot be used accurately to measure long path lengths.

Although the previous research has been focused on hot temperature and combustion applications, the same principles apply also to the measurements done in ambient air. One apparent application where good overlap, fast response, and good resolution are needed in temperature measurement is determination of the refractive index of air. Length measurement based on laser interferometry is practical and an accurate technique for dimensional metrology in a stable environment. The length scale is based on the wavelength of the laser which has to be calculated using the vacuum wavelength of the laser and the refractive index of the medium. Most measurements are done at atmospheric conditions where variation in the temperature, pressure, humidity, and CO_2 content affect the refractive index. In a well-controlled laboratory environment, these variations are in general low and measurement uncertainties in the order of 10^{-7}, or better, can be obtained. However, if measurements are done in an industrial environment or outdoors, fluctuations of ambient conditions can be several orders of magnitude larger, thus significantly increasing the measurement uncertainty. The acoustic method based on speed-of-sound measurement of an ultrasound burst signal can be also used to determine the effective air temperature with low uncertainty [7]. Echoes, beam spreading, and absorption, however, make it more suitable for shorter distances compared to the developed spectroscopic method.

This paper presents an experimental realization of a two-line room-temperature thermometer based oxygen A-band $b^1\Sigma_g^+ - X^3\Sigma_g^-$ weak transition near 762 nm. The thermometer is based on a simple and effective wavelength-multiplexed direct absorption method with amplitude modulation and normalized lock-in detection. Accurate and fast temperature measurement is demonstrated over 67 m absorption path. Rationale for the selected transitions is given, and general criteria for optimal line pair selection are discussed briefly. Two distributed feedback (DFB) lasers are used to scan two absorption transitions as well as the absorption free baseline that need to be measured to gain increased accuracy. The measurement system is designed to have a movable measurement head with fiber connections. The normalization scheme used in the setup effectively cancels small drifts in laser output power and interferences caused by the optics before the measurement head.

2 Theory

The transmission of light through an absorptive medium is governed by the Beer–Lambert law, which is given by

$$I = I_0 \exp(-\alpha), \tag{1}$$

where I is the transmitted intensity and I_0 is the initial intensity. The absorption coefficient α can be written as

$$\alpha = S(T)g(\nu, T, P)nl, \tag{2}$$

where $S(T)$ is the temperature-dependent absorption transition line strength, $g(\nu, T, P)$ is the normalized (area = 1) function which describes the shape of the absorption line at a given frequency ν, n is the molecular absorber number density, and l is the absorption path length. The total absorption spectrum of the medium is the sum of the spectra of individual molecular transitions. The absorption line-shape function is a function of temperature, pressure, and perturbing molecules (collision broadening). The line broadening effects can be divided into Doppler broadening and pressure broadening. Doppler broadening is dependent on the frequency, mass of the molecule, and on the temperature. At normal temperatures and at low pressures, Doppler broadening is the dominant broadening mechanism resulting in a Gaussian profile of the line-shape function. At atmospheric pressure, the dominant mechanism is pressure broadening. It results in a Lorentzian profile for the line-shape function which is quite close to a Gaussian profile near the center, but having a stronger absorbance far away from the line center. At the region where both broadening mechanisms contribute to the total profile, the line shape must be modeled using a Voigt profile, which is a convolution of Lorentzian and Gaussian profiles. The Voigt profile has been studied extensively, and many accurate analytical approximations have been developed [8,9].

The temperature-dependent absorption transition line strength can be expressed by

$$S(T) = S(T_0)\frac{Q(T_0)}{Q(T)} \exp\left[-\frac{hcE}{k}\left(\frac{1}{T} - \frac{1}{T_0}\right)\right] \times \left[\frac{1 - \exp\left(-hc\nu_0/(kT)\right)}{1 - \exp\left(-hc\nu_0/(kT_0)\right)}\right], \tag{3}$$

where $Q(T)$ is the total internal partition sum, E is the lower state energy, h is the Planck constant, k is the Boltzmann constant, and c is the speed of light [10]. The reference temperature, T_0, is 296 K. The center of the spectral-line transition frequency is denoted by ν_0. The third term in Eq. 2 accounts for the ratio of Boltzmann populations, and the last term for the effects of stimulated emission, which can be omitted in the visible wavelength region. For two separate absorption transitions having different lower state energies and sharing the same vibrational state, the ratio of the line strengths can be expressed as

$$R = \frac{S_1(T)}{S_2(T)} = \frac{S_1(T_0)}{S_2(T_0)} \exp\left[-\frac{hc\Delta E}{k}\left(\frac{1}{T} - \frac{1}{T_0}\right)\right], \tag{4}$$

where ΔE is the difference in their rotational state energies. Now the molecular absorber number density can be determined from the measured absorbances and the temperature can be deduced from the ratio of the absorbances using Eq. 4. The molecular number density is not required to determine the temperature if the scale is calibrated with reference temperature sensors, although it can be easily determined from the absorption measurements. The calibration is valid for all measurement devices using the same line pair.

3 Experimental Details

3.1 Line Selection

Fortunately, the center frequencies, line strengths, line-width parameters, and rotational energies for various common atmospheric molecules needed for accurate two-line thermometry are readily available from the HITRAN database [10]. Optimal line selection depends on whether only one laser is used or if it is possible to multiplex two or more lasers to the same absorption path. Additional lasers add complexity and price, but also improve the achievable sensitivity. A single laser limits the available wavelength range, which usually leads to a compromise when selecting lines with high R. The availability of DFB lasers at different wavelengths is also a limiting factor when choosing line pairs in an experimental realization of two-line thermometry. Absorbance of the two lines should be comparable and the absorption over the desirable path length should be in ideal case tens of percents. If the absorbance is higher, the saturation property of Eq. 1 decreases the achievable temperature sensitivity. At low absorbance levels, noise becomes a significant degrading factor to the overall performance. Within the tuning range of the used diode(s), there should be a free spectral window ideally with zero absorbance, which could be used to provide baseline information on internal losses and non-idealities of the system. Free spectral windows are practically nonexistent at ambient conditions when the medium is standard air, but there are still regions where the absorbance is low enough to allow measurement of the baseline with low uncertainty.

The A-band of oxygen near 762 nm is well-suited for two-line thermometry near room temperature at atmospheric pressure. Compared to water, which has multiple strong features in visible and near-IR regions, the oxygen mole fraction can be assumed to stay relatively stable when temperature, humidity, or pressure vary. The A-band has a selection of well-isolated transitions with weak and strong absorbances, making it good for both short- and long-range applications. The band is also practically free from interfering molecular absorptions. Water and hydroxide have some transitions in the region, but they are either out of band or several orders of magnitude weaker than oxygen transitions at standard atmospheric concentrations. Furthermore, high performance DFB and VCSEL lasers are available at this range, thus making it possible to build compact and cost effective measurement systems. The simulated absorption

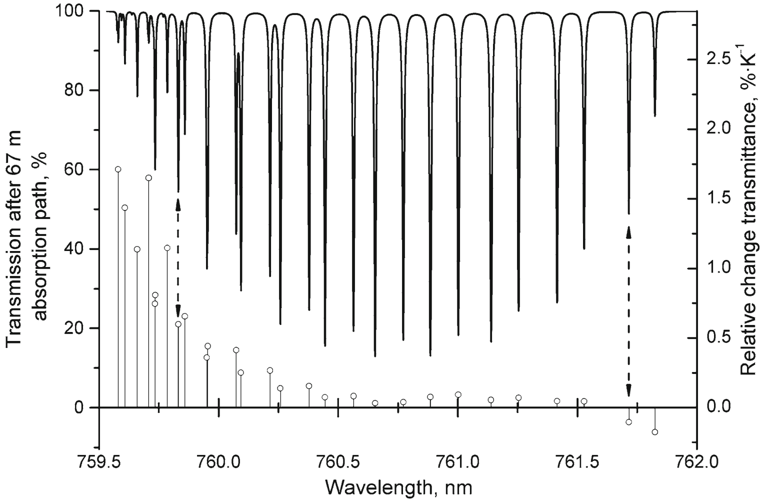

Fig. 1 Oxygen A-band absorption spectrum for a 67 m path in ambient air and relative change in absorption for each transition. Used transitions are marked with *dashed double arrows*

spectrum of the oxygen R-branch is shown in Fig. 1 for a path length of 67 m at standard pressure and temperature (20 °C, 1 atm., 20.95 % O_2). The Voigt profile is used as the line-shape function using an approximation adopted from [8]. The Lorentzian halfwidths are calculated using air broadened halfwidths γ_{air} from HITRAN and by using an approximate equation from [9]. The relative change in absorption for a 1 K increase in temperature is presented for each transition. It can be seen from the figure that the saturated transitions in the middle are not suitable for high sensitivity thermometry when using a 67 m path length. The theoretical sensitivity is $\sim 0.7\,\% \cdot \text{K}^{-1}$ for the transition marked in the figure, which takes into account the saturation caused by the Beer–Lambert law. The marked transitions are R19-Q20 at 759.831 nm and R1-Q2 at 761.715 nm using HITRAN notation.

3.2 Measurement Setup

The experimental setup is shown in Fig. 2. Two DFB lasers (Eagleyard photonics) are mounted in a thermoelectric cooler used for temperature stabilization. The nominal wavelength for DFB 1 and DFB 2 are 760.7 nm and 761.6 nm, respectively. The tuning range (temperature) for both lasers is ∼±1 nm around their nominal wavelengths, making it possible to use almost any line shown in Fig. 1. The half-wave plates before the beam multiplexing are used to match the polarization state of the DFB to the input of the electro-optic intensity modulator (EO-IM, ConOptics). Beam shaping is used to optimize the beam that is focused into a single-mode optical fiber. The light is guided to the measurement head that is located in another laboratory. The output radiation of the fiber is collimated using an achromatic doublet lens (75/f:1.5), which produces a 25 mm low divergence output beam. Part of the output beam is immediately reflected back using a wedged metallic beam splitter. A silicon photodiode (PD B) provides

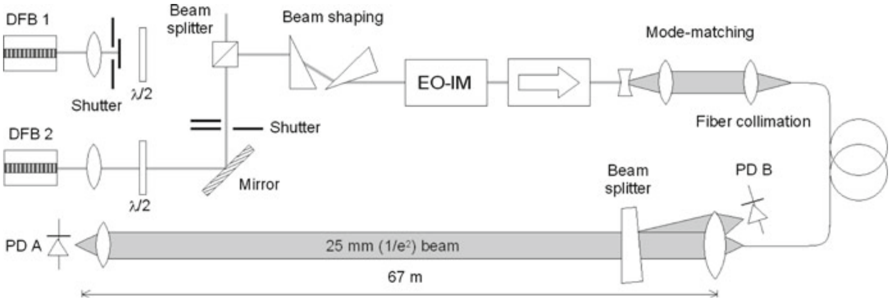

Fig. 2 Schematic of two-line thermometry measurement setup when DFB 2 is active

the reference signal for normalization. The actual absorption is measured with silicon photodiode A (PD A). The optical power at the PD A is ~1 mW. EO-IM is modulated at 1.4 kHz, and two lock-in amplifiers (SR830) measure the lock-in signal. Each temperature measurement requires a measurement of both absorption peaks and the baseline. The baseline is measured using DFB 2, which is temperature tuned to the free transmission window shown in Fig. 1 just left of the transition used in thermometry. Both lasers are current tuned after each measurement to the center of the absorption peak to compensate for small drifts in electronics or caused by thermal effects. The system is fully automated using Labview software and a data acquisition card.

4 Sensor Demonstration

Temperature measurement is a three-step process. First, the frequency of the DFB 2 is swept by current over the R1-Q2 transition and the peak absorption is determined. Immediately after the sweep, the temperature of the DFB 2 is adjusted to the absorption-free part of the spectrum. Next, the frequency of the DFB 1 is swept over the transition R19-Q20 to determine the corresponding peak absorption. Finally, the frequency of the DFB 2 is swept over the absorption-free part to obtain the baseline for both absorption peaks. The total measurement time for one temperature measurement is close to 60 s. Figure 3 shows a typical result measurement of step one and three using DFB 2. The measurement result from step two is left out for clarity. The time constant of the lock-in amplifier was 30 ms, and the time between consecutive points was ~50 ms. The frequency sweep of both lasers is set to correspond to approximately ~0.5 % of the height of the absorption line. The width of the sweep is sufficient to determine the peak value of the absorption line and to allow loose frequency stabilization of the lasers by adjusting the current so that the center of the sweep matches with the line center. A moving average of ten points was used to smooth the data before determining the peak absorption. This causes a small error in the peak value, but the error can be neglected as the measurement is based on a ratio measurement of the two peaks. The small offset is practically the same for both peaks, and we found that the shape of the peaks remained the same over the measurement period of one hundred hours. In theory, a continuous baseline measurement is not necessary in two-line thermometry, but we discovered that the statistical noise of our measurement

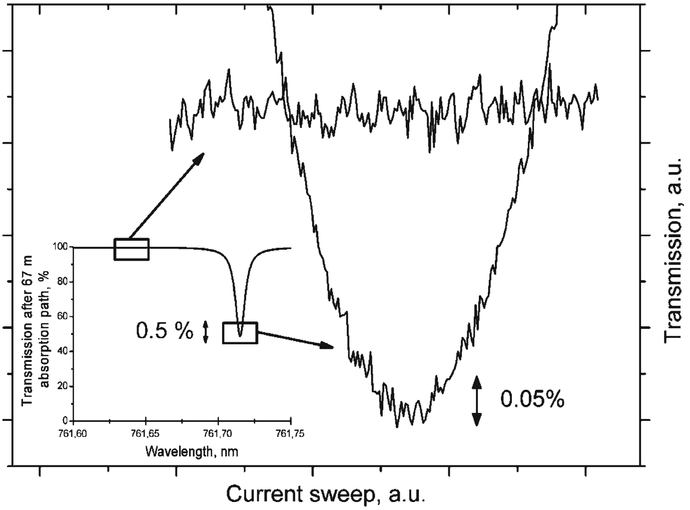

Fig. 3 Typical measurement result of the R1-Q2 transition and the baseline. Two *squares* in the inset are exaggerated for clarity. Portion of the absorption peak height is marked with *vertical double arrows* for scale

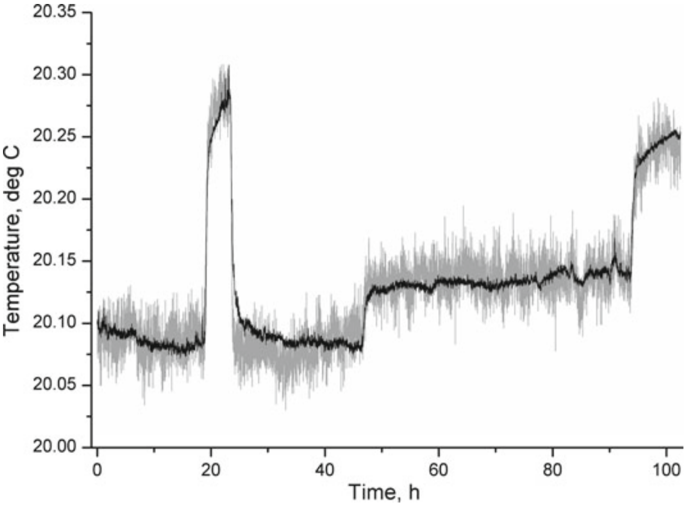

Fig. 4 Result of a 100 h temperature measurement. Raw spectroscopic data are marked with a *gray line*, and an average of seven conventional temperature sensors is marked with a *black line*. Observed temperature changes are made intentionally

system was lower when the baseline information was used. For example, if the ratio R is 1.1, which is close to the ratio of the chosen line pair, a 0.5 % negative offset in the baseline increases the ratio by 0.056 % which is equal to a significant 39 mK increase in temperature.

Raw temperature-measurement data, including all measurement points, for a 100 h measurement period is shown in gray in Fig. 4. The measurement path is placed over a 30 m long interferometric measurement rail designed for calibration of electronic distance measurement instruments, measuring tapes and poles, and circometers. The laboratory where the 30 m measurement rail is located is approximately 40 m long. To increase the measurement path length, a mirror and double-pass scheme is used to obtain the total 67 m measurement path. We use seven fast conventional temperature sensors distributed evenly over the length of the measurement path as a reference instrument. In principle, the absolute temperature scale could be obtained from the tabulated spectroscopic data. However, the experimental uncertainty in the HITRAN database, which is usually on the order of a few percent for line strength, causes a significant error and therefore the temperature scale is obtained from the reference thermometer. The black line is the average of seven sensors each averaged over 1 s. The laboratory where the measurement was performed has very good temperature control with an adjustable set-point. To investigate the performance of the spectroscopic temperature measurement, we have made step changes to the set-point, that very rapidly affect the temperature of the incoming air. The first step-response test (after 20 h of continuous measurement) was performed to investigate the response speed of the spectroscopic measurement as compared to conventional sensors. There is a significant difference in the response speed, especially when the temperature is adjusted back to the original setting. As expected, the spectroscopic method is much faster compared to the conventional sensors even in the case of a small temperature step to which the conventional sensors react rapidly. The 200 mK step can be considered quite common or even small in environments that are not well temperature controlled. The second and third step-response tests were performed to assess the sensitivity of the system to small temperature changes. The $\sim$40 mK step can be easily resolved, and the calculated RMS noise of the temperature measurement is 22 mK, which may be partially due to actual temperature fluctuations of the air. An empirical pressure correction of $-45\,\mathrm{mK} \cdot \mathrm{mbar}^{-1}$ was used to cancel the variations caused by changes in the ambient pressure.

5 Conclusions

Two-line spectroscopic thermometry has been previously used mainly in high-temperature applications. In this work, we have demonstrated that oxygen can be used as a probe to measure temperature over a relatively long path at normal ambient conditions. The selection of the two absorption lines is discussed, and optimal lines are chosen for the 67 m path length. Well-separated absorption peaks, absorption-free transmission windows, strong- and weak-line strengths, stable concentration, and good sensitivity for temperature changes make oxygen a good choice for a probe molecule. Two DFB lasers were used as laser sources capable of operating at virtually any wavelength of interest thus making it possible to vary the path length while maintaining good sensitivity. We have demonstrated a measurement configuration based on lock-in detection and normalization. A separate measurement head with a fiber connection simplifies measurement arrangements. We have shown that the developed measurement system is capable of measuring rapid changes and small variations in temperature, which are required, for example, in optical dimensional measurements to compensate for the temperature dependence of the refractive index of air. The RMS noise of the demonstrated measurement system is 22 mK, which corresponds to $\sim 2 \times 10^{-8}$ RMS noise in the refractive index of air.

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