

STUDY OF IN-SITU GAS SENSOR BASED ON MILLIMETER / SUBMILLIMETER WAVE SPECTROSCOPY

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1. INTRODUCTION

The millimeter and submillimeter wave bands are abundant in absorption and radiation spectrum of gases. Whereas these bands have been extensively utilized in the radio astronomy, space borne radiometry and high altitude atmospheric analysis [1], the application in industry, especially of the submillimeter wave, has been explored only to a limited extent and remained to be a terra incognita. Yet, the prospects are well as witness the work of Brand et al. who demonstrated conspicuous 600GHz band radiometric images of plant leaves [2]. Further, the recent advancement of vector signal processing above 100GHz up to terahertz frequency and reliable mixer/receiver will open the opportunity for industrial in-situ gas sensors based upon the principle of millimeter / submillimeter wave spectroscopy [3]. The in-situ gas sensor is vital to establish a modern and efficient air pollution control process and plasma gas synthesis of new materials such as super carbon. A conceived gas process integrated with the in-situ gas sensor is depicted in Fig. 1. The RF signal generated by a coherent source is fed into the open cavity which is conformed in the active gas region, and the vector of the received signal is analyzed to determine the gas condition such as the concentration.

Such gas sensor will be attractive because of gas selectivity, multiple parametric measurement such as gas

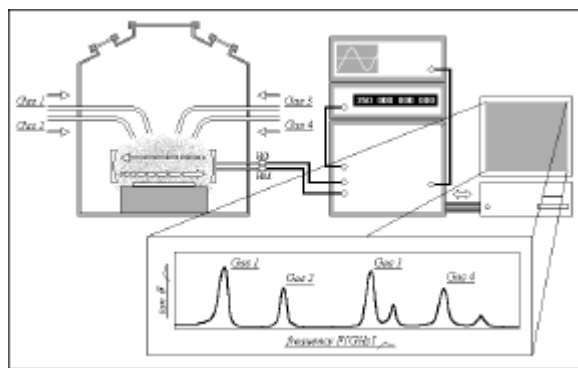


Fig. 1. Concept of in-situ gas sensor.

concentration, temperature and pressure, and of the in-situ measurement capability. The gas selectivity, due to the inherent and discrete distribution of absorption and radiation spectrum of gases, enables the analysis on a specific gas element without interference from other coexisting constituents. By the same token, various gas constituents can be measured simultaneously. The parameters such as concentration, temperature and pressure can be measured as the corresponding change of the absorption spectrum. As an example, the parametric study of the well known 50-70GHz oxygen complex reveals that at 60GHz, the increase of temperature from 293K to 303K results in the decrease of the gas absorption coefficient by 1dB, the higher shift of peak absorption frequency by 20MHz, and the increase of the bandwidth by 0.24GHz. These resultant changes are well within the capability of modern phasor measurement. The in-situ measurement is realized by passing the radio wave through

the spatially extended active region of gas, so as to observe the constituents as they populate, in sharp contrast to the conventional gas sensors. Based upon these background and our previous work [4]-[6], this paper will discuss the following subjects.

- (1) The parametric study based on the empirical formula of oxygen spectra with the variable of the temperature and pressure for a given fixed density is introduced. And new spectrum diagram to explicitly delineate the result of the parametric study is proposed.
- (2) The evaluation of the proposed scheme of the gas sensor has been conducted at 60GHz-band and 118GHz band oxygen spectra.

2. PARAMETRIC STUDY of 60GHZ BAND OXYGEN SPECTRUM

Rosenkranz has derived the characteristic formula of oxygen spectra based on the measured spectrum [7]. The absorption coefficient k_{O_2} is shown by the following expression.

$$k_{O_2} = 3.71 \times 10^{-6} f^2 \frac{P}{1013} \left(\frac{300}{T} \right)^2 F' [m^{-1}] \quad (1)$$

where F' is the line shape function [Hz], f is the frequency [GHz], T is the temperature [K], P is the pressure [hPa]. The parametric study with the variable of the temperature and pressure for a given density using Eq. (1) is discussed in the following. The spectrum changes as a function of temperature and pressure are shown in Fig. 2. The intensity increases with the pressure, but decreases with the temperature ($3 \times 10^{-6} Np / m \cdot hPa$, $-2 \times 10^{-5} Np / m \cdot K$). The half-maximum bandwidth increases both with the temperature and the pressure (9MHz/K, 0.6M/hPa).

3. SPECTRUM DIAGRAM

A new diagram to explicitly delineate the result of the parametric study with the variables of the temperature and pressure for a given density is proposed and presented over the range of 150-600K and 500-2000hPa.

The procedure is epitomized as follows. The first, a topography is formed with the temperature on the transverse axis, and the pressure on the longitudinal axis, and the intensity as the height contour. The second topography is formed for the half-maximum

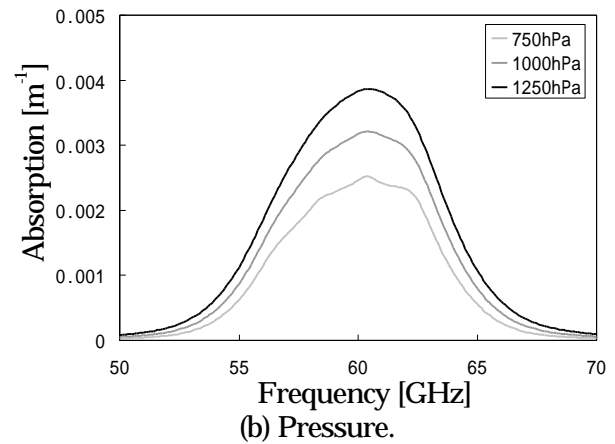
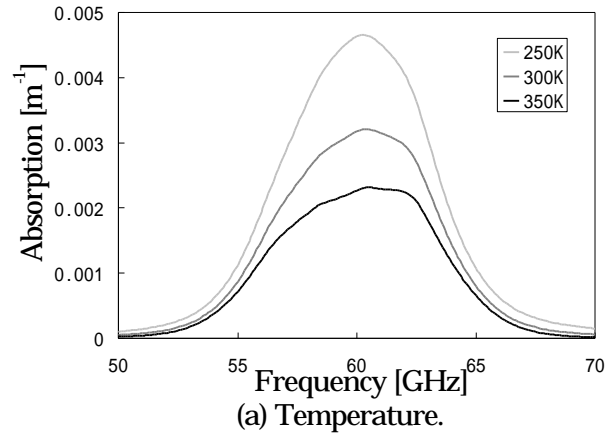


Fig. 2. Parametric study of 60GHz band oxygen spectrum.

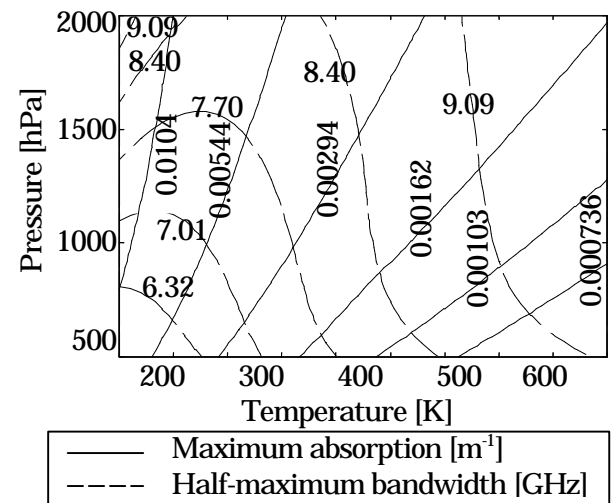


Fig. 3. 60GHz band oxygen spectrum diagram.

bandwidth on the height contour on the same plane as the first graph. Finally, in order to reversibly obtain the temperature and the pressure for a given set of intensity and half-maximum bandwidth, the two topographies are superposed into one chart. The resultant spectral diagram as Fig. 3 explicitly represents the relationship between the set of temperature and pressure and the set of intensity and half-maximum bandwidth. Referring to this new diagram, the temperature and the pressure can be directly read from the cross point of the height contours corresponding to the measured values of intensity and half-maximum bandwidth. For instance, when the maximum absorption and half-maximum bandwidth are $(0.002\text{m}^{-1}, 8.40\text{GHz})$, then the temperature and pressure are $(370\text{K}, 1470\text{hPa})$.

4. MEASUREMENT of OXYGEN SPECTRUM

(1) Fabry-Perot resonator absorption cell coupled with vector measurement

Historically, the instrument of gas spectroscopy, for example in the case of oxygen measurement conducted first by Beringer in 1946, consisted of klystron and crystal multiplier, modulator, waveguide absorption cell, and crystal detector for intensity measurement [8]. Then in 1971, Hrubesh et al. replaced the long cell by a high Q Fabry-Perot resonator with the effective absorption path length and large volume-to-surface ratio, giving a distinct advantage over the waveguide cell [9]. On the track of this scheme, it is expected further improvement to replace the transmitter and receiver with a vector measurement, so as to realize more accurate and higher resolution spectrum measurement as well as much compact and easy-to-handle features.

The quality factor of Fabry-Perot resonator filled with absorbing gas is defined as $1/Q = 1/Q_0 + 1/Q_g$. Here Q_0 is unloaded

Q , and $1/Q_g$ represents losses in absorbing gas as related as $1/Q_g = \tan d$.

(2) Necessity of vector measurement system

Vector locus of Fabry-Perot resonator is shown in Fig. 4. A leak, coupled between coupling holes, is indicated as \vec{OL} in the vector form. Accordingly, the starting point of resonance vector shifts from O to L , and the resonance point R does not agree with the maximum distant point M from the origin O . Because of this reason, a vector measurement system is required to achieve higher accurate spectrum measurement.

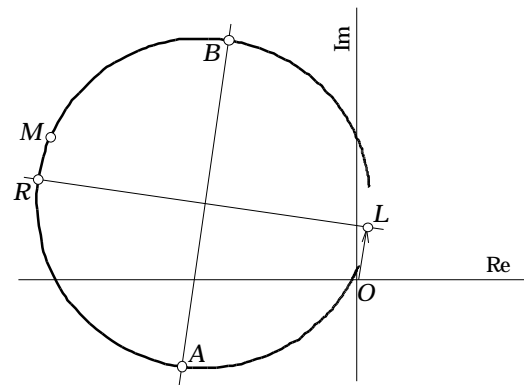


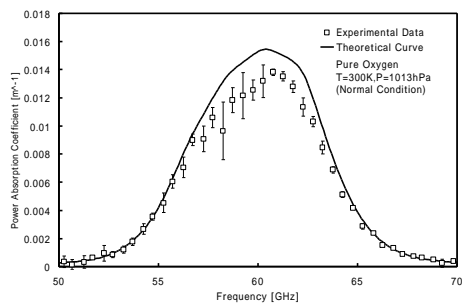
Fig. 4. Resonance vector locus.

(3) Measurement

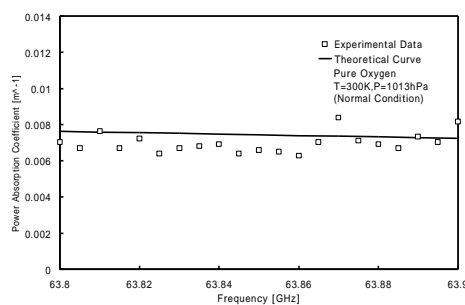
The measurement setup consists of Fabry-Perot resonator absorption cell and vector measurement system. Fig. 5 is a set of measured oxygen absorption spectrum.

For the 60GHz band measurement in Fig. 5(a), the data shows a little variation as a whole. Especially for the 50-57GHz band and 64.5-70GHz band, the data is in good agreement with the theoretical value. It is noted in Fig. 5(b) that the resolution of 5MHz is achieved at the 63.8GHz band. From the result of the parametric study, 5MHz resolution for the half-maximum width will correspond to the resolution of 0.74K or 7.1hPa at $(300\text{K}, 1000\text{hPa})$. The result at 118GHz band shown in Fig. 5(c) is Lorentzian shape as expected. The integrated intensity is $6.57 \times 10^6 \text{m}^{-1}\text{Hz}$ that is smaller than the

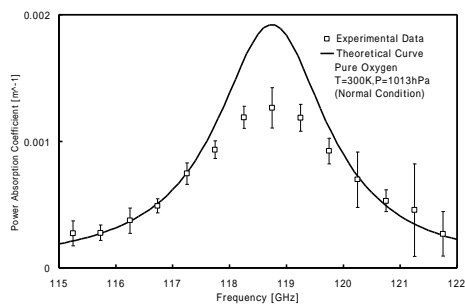
theoretical value $7.17 \times 10^6 \text{ m}^{-1} \text{ Hz}$. The half-maximum width is 3.25GHz that is wider than the theoretical value 2.4GHz. The reason for them is under examination.



(a) 50-70GHz spectrum.



(b) 63.8GHz spectrum.



(c) 118GHz spectrum.

Fig. 5. O_2 absorption spectrum.

5. CONCLUSION

The parametric study with the variable of the temperature and pressure for a given density based on the empirical formula is at first discussed, and then the spectrum diagram that represents the change of the spectrum with temperature and pressure is derived.

The experimental examination of the proposed spectroscopic system is conducted at the oxygen 60GHz band and 118GHz band, and the result at 60GHz band shows good accuracy and resolution.

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