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Theoretical analysis of off beam quartz-enhanced photoacoustic spectroscopy sensor

Hongming Yi [a,b], Kun Liu [a,b], Shanwen Sun [a,b], Weijun Zhang [a,b], Xiaoming Gao [a,b,*]

[a] Key Laboratory of Atmospheric Composition and Optical Radiation, Chinese Academy of Science, Hefei 230031, China
[b] Laboratory of Atmospheric Physico-Chemistry, Anhui Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, Hefei 230031, China

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ABSTRACT

Off beam quartz-enhanced photoacoustic spectroscopy (OB-QEPAS) sensors are based on a recently developed approach to off-beam photoacoustic (PA) detection which employs a quartz tuning fork (QTF) as an acoustic transducer. A microresonator (mR) with a side slit in the middle is used to enhance PA signal. This paper describes a theoretical model of an OB-QEPAS-based sensor. By deriving the acoustic impedances of the mR at two ends and the side slit in the middle in the model, we obtain a formula for numerically calculating the optimal mRs' parameters of OB-QEPAS-based sensor. We use the model to calculate the optimal mRs' lengths with respect to the resonant frequency of the QTF, acoustic velocities inside mRs, inner diameters of mRs, and acoustic conductivities of the mRs' side slits, and found out that the calculated results closely match experimental data. We also investigated the relationship between the mR selected in "on beam" QEPAS, OB-QEPAS, and an acoustic resonator (AR) excited in its first longitudinal mode used in conventional photoacoustic spectroscopy (PAS).

1. Introduction

Laser photoacoustic spectroscopy (PAS) [1,2] is a well established method used in trace gas sensing applications, which is based on detecting acoustic waves generated by a medium absorbing modulated optical radiation as a result of photoacoustic (PA) effect. A sensitive acoustic transducer is used to detect PA signal. Up to date, due to the alternative acoustic transducers, broadband microphone based conventional PAS [3], quartz-enhanced PAS (QEPAS) [4], micro electro-mechanical systems (MEMS) scaled PAS (MEMS-scale PAS) [5], newly developed PAS used electromechanical films (EMFIT) as acoustic transducer (EMFIT based PAS) [6] and silicon cantilever enhanced PAS [7] have been demonstrated and widely used for trace gas detection. Actually, our research purpose is to acquire higher sensitivity and more compact system configuration of PAS-based sensor. As a result, research committed to further improve the sensitivity of PAS-based sensor has followed schematically three lines: use of new light sources, design of different resonant cell types with optimized geometry, and improvement of data analysis. In particular, designing optimum resonant PA cells in traditional PAS to improve the signal to noise ratio (SNR) was verified to be a very effective method through the former theoretical analysis and experiments measurements [8–12]. Conventional microphone based PAS with optimized resonant PA cell has been acquired very high sensitivity and employed to widespread applications [1–3,8–12].

Quartz-enhanced photoacoustic spectroscopy (QEPAS) is a newly developed sensor technology which firstly introduced by A.A. Kosterv in 2002 [13]. In combination with various light sources, such as diode laser or laser diode (DL or LD), optical parametric oscillators (OPO), interband cascade lasers (ICLs) and quantum cascade lasers (QCLs), QEPAS has been successfully applied to the detection of various simple molecules with narrow absorption spectra [14–16] and larger molecules with broad, unresolved spectral absorption features [17–19]. Analogous to traditional microphone based PAS, it is a very effective method to design and optimize acoustic microresonator (mR) for further improving the sensitivity of QEPAS-based trace gas sensor [20,21]. As a result, recently, four typical QEPAS spectrophones configurations [21] have been reported, which referred to "bare QTF QEPAS", on beam QEPAS, half on beam QEPAS, and off beam QEPAS (OB-QEPAS), respectively. The reported OB-QEPAS-based sensor configurations include a spectrophone (the module for detecting laser-induced sound) consisting of a QTF and a microresonator composed of a tube with a side slit in the middle [22,23]. Experiments have shown that OB-QEPAS yields a SNR gain ~19 compared to "bare QTF QEPAS" [23]. But for on beam QEPAS with the optimum mR parameters, its SNR gain can be as high as ~30 compared to "bare QTF QEPAS" [16,20,21]. Comparing the SNR gain of OB-QEPAS to that of on-beam QEPAS

* Corresponding author at: Chinese Academy of Science, Key Laboratory of Atmospheric Composition and Optical Radiation, Hefei 230031, China.
Tel./fax: +86 551 5591534.
E-mail address: xmgao@aiofm.ac.cn (X. Gao).

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spectrophone design, the optimum OB-QEPAS design has a 1.6–1.7 weaker SNR gain at atmospheric pressure [23]. However, technologically, OB-QEPAS is more flexible, easier to assemble and align regarding configurations between QTF and mR, as the excited light source no more pass through the smaller gap between the prongs but directly through the mR to avoid obstruction of the used excitation radiation. Especially, for real application, OB-QEPAS spectrophone design makes it possible to have the advantage to use light sources with lower beam quality. For example, broadband blue laser diode based OB-QEPAS was developed for trace NO_2 detection [19], light emitted diode was used as excited source for O_3 measurements with OB-QEPAS [24], and OB-QEPAS was adopted to measure the alignment-dependent energy dumped into gaseous linear molecules (O_2, N_2, CO_2 and CO) [25]. Those examples all used light sources with low beam quality as PA excited sources. These advantages make OB-QEPAS spectrophone configuration to become as important as "on beam" structure. However, former works [22,23] mainly focused on experimental study and the systematical theory for OB-QEPAS was not given. So that it is necessary to analyze OB-QEPAS spectrophone theoretically for designing and optimizing OB-QEPAS-based sensor.

In this paper, we describe a theoretical model for OB-QEPAS-based sensor currently proposed by Kun Liu et al. [22,23]. This theoretical model was used to calculate the optimum mR lengths with respect to different acoustic velocities, various inner diameters (IDs), outer diameters (ODs) and the side slits of mRs. The model was validated by comparison theoretical calculations with experimental results cited from [22,23]. Our model shows that the theoretical calculations and experimental measurements are in very good agreement. The influence of acoustic velocity on OB-QEPAS-based sensor performance was also investigated. Finally, the relationship between the mR used in OB-QEPAS and on beam QEPAS and acoustic resonator (AR) excited in its first longitudinal mode adopted in conventional microphone based PAS was analyzed and discussed.

2. Theoretical model

OB-QEPAS spectrophone consists of a QTF and a so-called mR (shown in Fig. 1(a) and 1(b)). The mR is formed by one tube with a side slit in the middle (shown in Fig. 1(c)), and the QTF is coupled to the mR by putting it outside the mR tube near the opening of the side slit to probe the acoustic vibration excited in the gas contained inside the tube [22,23] (shown in Fig. 1(a) and 1(b)). Being different from conventional microphone with response frequency of 20–20,000 Hz, the QTF is used as an acoustic transducer with a fixed response frequency of $f_0 \sim 32.768$ kHz, and the mR with a side slit in the middle is selected for accumulating the acoustic wave energy inside the mR tube. The length (l_0) and width (w_0) (l_0, w_0, see Fig. 1(c)) of the side slit are chosen to well couple acoustic energy into the gap between two QTF prongs with a width of 0.3 mm (shown in Fig. 1(a)). Microresonator center is positioned below the QTF tips, and the distance from the QTF tips to the mRs' axis is 0.7–1.0 mm [22,23,26] (shown in Fig. 1(b)). In order to improve the sensitivity of OB-QEPAS-based sensor, a modified mR (shown in Fig. 1(d)) was made to reduce the viscous drag [27,28] between the mR and the QTF so as to keep the QTF assembled into OB-QEPAS spectrophone to work with a high Q factor ($Q \sim 8000$), because the subsequent signal to noise ratio (SNR) of the sensor is directly proportional to $\sqrt{Q}$. But the modification to mR for forming the modified mR does not change the basal acoustic characteristics of the mR tube. And the resonant frequency of the mR with a side slit in the middle is noted as f_{mR}. The optimum OB-QEPAS spectrophone configuration is to make acoustic coupling between QTF and mR to be the best, namely sets $f_{mR}=f_0$. Therefore, in real applications, designing optimum mR parameters to keep $f_{mR}=f_0$ is an effective method to acquire the best sensitivity of OB-QEPAS-based sensor. In the following section, a theoretical model will be presented to give a method to obtain the optimum mR parameters of this "off beam" configured sensor.

In the case where the cross-sectional dimensions of an acoustic resonator are much smaller than the acoustic wavelength, the excited acoustic wave can be described by a one-dimensional acoustic field along the length of the resonator [10]. In QEPAS, the used mR (with a diameter ≤ 1.50 mm in comparison with an acoustic wavelength of $\lambda \sim 10.5$ mm at atmosphere and room temperature) can thus be treated as a one-dimensional acoustic resonator, only the first longitudinal acoustic resonance occurs inside the mR tube. Presently, there are mainly six prototypes of one-dimensional acoustic resonator to be usually used in acoustic instruments (shown in Fig. 2(a)–2(f)), which refer to open–open tube (Fig. 2(a)), close–close tube Fig. 2(b), open–close tube (Fig. 2(c)) [10]; open–open tube with an orifice in the middle (Fig. 2(d)), wide open–partly open tube (Fig. 2(e)), full close–partly open tube (Fig. 2(f)) [29,30], respectively. In the later sections, we will investigate the acoustic impedance at two open ends and the side slit of open–open tube with a side slit (treated as an orifice) (shown in Figs. 2(d) and 3(a)) in the middle used in OB-QEPAS for theoretical analysis of the resonant condition of

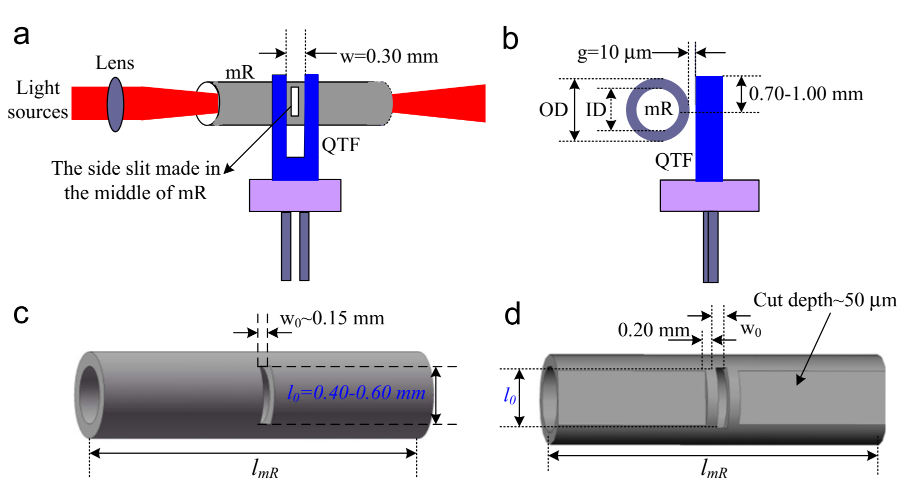

Fig. 1. Configuration of OB-QEPAS spectrophone and the used mR tube. OB-QEPAS spectrophone profile: (a) seen from the side slits of the mR; (b) seen from the mR' axis; (c) the 3D (3 dimensions) map of the mR tube with a side slit in the middle; (d) the 3D map of the modified mR.