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Optimization of spectrophone performance for quartz-enhanced photoacoustic spectroscopy

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A B S T R A C T

We numerically investigate the effects of spectrophone parameters, including the operating acoustic frequency, the relative position of the quartz tuning fork and the excitation laser beam, the gap between the resonant tubes and the tuning fork, and the diameter and length of the resonant tubes, on the performance of gas sensors based on quartz-enhanced photoacoustic spectroscopy. A pair of rigid tubes with inner diameter of 0.2 mm and length of 5.1 mm, placed 0.6 mm down from the opening and 20 μm away from the edge of the tuning fork, is suggested for optimal performance.

1. Introduction

Quartz-enhanced photoacoustic spectroscopy (QEPAS), in which periodic light absorption is converted into a localized acoustic pressure wave through photoacoustic (PA) effect and the pressure wave is detected with a tiny quartz tuning fork (QTF), has been demonstrated for trace gas detection with outstanding performance [1,2]. To further enhance the PA signal, a pair of rigid tubes, one on each side of the QTF facet (Fig. 1), was introduced, which acts as an acoustic microresonator (mR) to amplify the acoustic signal [3–5]. An enhancement factor as high as 30 was achieved by properly selecting the dimensions of the tubes [6]. Early work used two resonant tubes with a total length around half of the acoustic wavelength λ_S in gas, to form an antinode in the middle of the tubes [2]. Later experiments showed that a larger PA signal can be obtained by using a mR with each of the tubes having a length of around $\lambda_S/2$, because the gaps between the tube facets and tuning fork surfaces make the acoustic mode in each of the tubes relatively independent from each other [5]. Further detailed studies revealed that tube length for achieving optimal performance is somewhere between $\lambda_S/4$ and $\lambda_S/2$ [6,7], and the size of the gaps significantly affects the acoustic coupling between the tubes. Dong et al. [6] carried out experimental investigations on spectrophone optimization, but the samples are limited that it prevents a comprehensive investigation being carried out. Multiple parameters, including length and inner diameter (ID) of the tube, gap between the tube and tuning fork, gas pressure, dimension of the tuning fork, could play important roles on the acoustic coupling and consequently the PA signal, and the relationships among them are not straightforward.

To better understand the acoustic coupling between the mR and tuning fork, and to optimize the performance of the spectrophone, we report a numerical model based on COMSOL Multiphysics software with finite element method [8]. With this model, the influence of acoustic frequency, tuning fork position, and tube dimensions on the acoustic coupling and pressure distribution, and hence the generated acoustic signal are studied, and a set of parameters for optimal spectrophone performance is identified.

2. Numerical model

As the physical processes involved in QEPAS are complicated and no simple analytical model can be applied, we developed a numerical model based on the COMSOL software. Two modules, pressure acoustics and piezo solid, are used for investigating acoustic coupling and piezoelectric effect of QTF respectively. Considering the symmetry of the mR and QTF, only half of the tuning fork (marked in blue) and the resonant tubes (marked in red) are included in our numerical model, as shown in Fig. 2. The boundary of gas involved is assumed to be of a spherical shape and an outer spherical shell is introduced as the perfectly matched layer (PML) to absorb the reflected acoustic wave from the boundary. Considering that the diameter of the light beam through the resonant tubes is relatively small (~0.05 mm at waist [9]) compared to the gap between the QTF prongs (0.2 mm) and the ID of the tubes (typically ≥0.2 mm), the acoustic pressure wave may be regarded to be originated from

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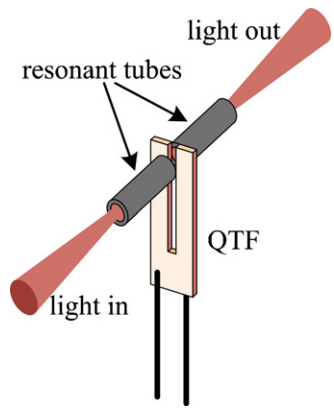

Fig. 1. Schematic of a QEPAS spectrophone comprising of a tuning fork and two rigid resonant tubes. Light is focused though the tubes and the gap between the two prongs of tuning fork.

a line source along the axis of the tube and propagate all around. The source term setting in COMSOL is given by [10]:

$$iS = i\frac{(\gamma - 1)\alpha P_0}{\rho_0 c_S^2}, \tag{1}$$

where i is the sign of imaginary part, γ is the adiabatic coefficient of target gas, ρ_0 and c_S are the gas density and the sound velocity in the gas, respectively, α is the light absorption coefficient of the gas, and P_0 is the laser power. In our simulation, the gas involved in the model is assumed to be at atmospheric pressure.

The dimension of the QTF (Raltron R38) used in this model is the same as in [11], i.e., 3.636 mm × 0.54 mm × 0.232 mm for each prong and 0.2 mm for the gap between the two prongs. To better match the actual structure, the base of the QTF that is exposed to the gas is subdivided into a fixed section with a length of 2 mm and a free section with a length of 0.1 mm with rounded corner. The QTF subdomains are only active in the piezo solid module, resonant tubes are assumed to be rigid and not active, while the other subdomains are active in the pressure acoustics module. The detailed subdomain and boundary setting can be found in Ref. [10]. The acoustic pressure applied to the tuning fork prong excites mechanical oscillation of the QTF, which results in the

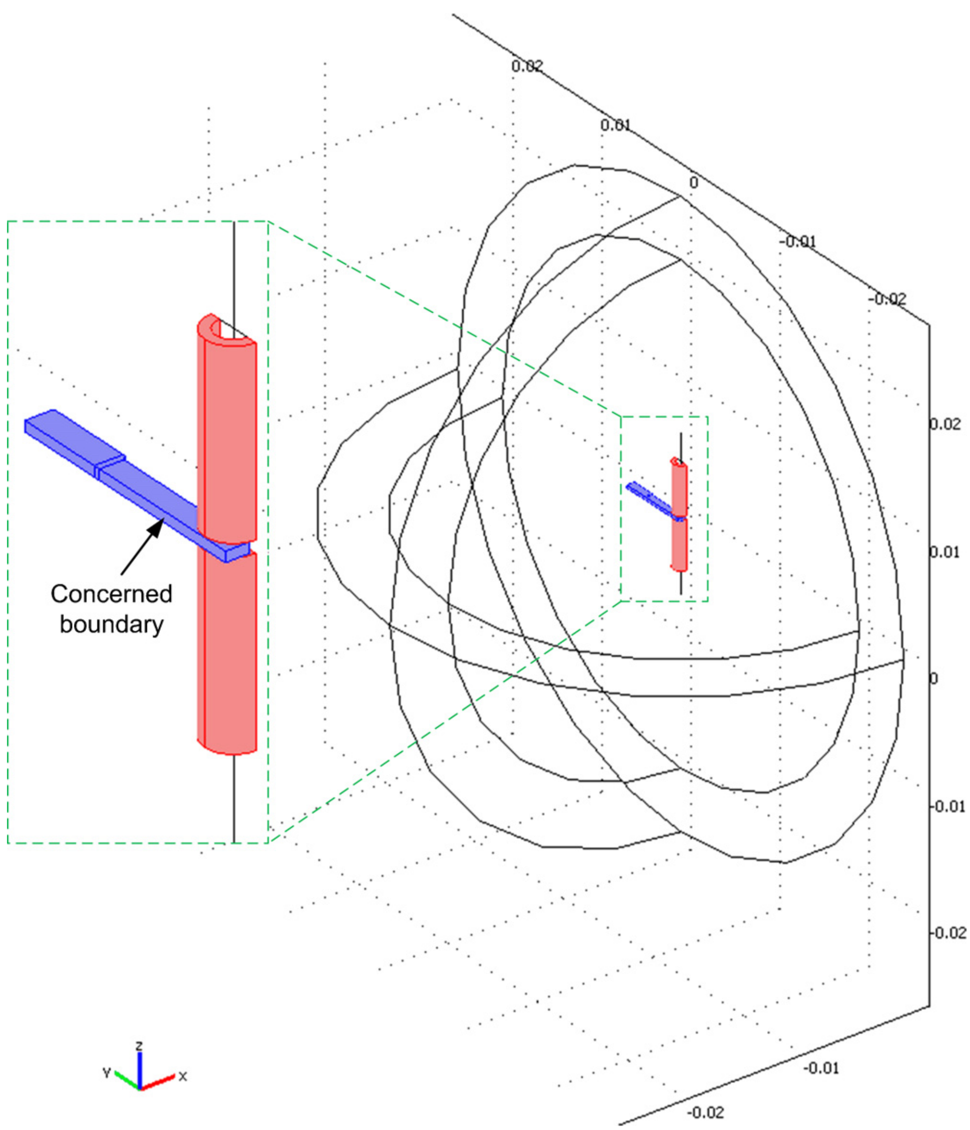

Fig. 2. Numerical model for spectrophone optimization. The red domains are resonant tubes and the blue ones are QTF. The unit of scale is meter. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)