Numerical and Experimental Investigation for a Resonant Optothermoacoustic Sensor

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Abstract: A theoretical study of a resonant optothermoacoustic sensor employing a laser source and a quartz tuning fork receiver validates experimental results showing that the source should be positioned near the base of the receiver.

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1. Introduction

Cost-effective sensor systems with the ability to identify trace gases with sensitivities in the ppm to ppb range are becoming essential tools for environmental monitoring, medical diagnostics, and homeland security. Quartz-enhanced photoacoustic spectroscopy sensors (QEPAS) hold great promise for such sensor systems because of their simple design, compact size, and potentially low cost [1], [2]. Recently, Kosterev *et al.* [3] proposed a related sensing method – resonant optothermoacoustic detection (ROTADE) – which could further increase wavelength selectivity and sensitivity. Like QEPAS sensors, ROTADE sensors employ a quartz tuning fork (QTF) as a resonant transducer. With the ROTADE technique there is the possibility of performing measurements at lower pressure than for QEPAS sensor, which allows for higher spectral resolution.

As in the case of QEPAS, to detect the presence of a trace gas, a modulated laser beam is directed between the tines of a QTF. The interaction of modulated laser radiation with a gas results in periodic heating and cooling. Whereas QEPAS relies on the conversion of thermal disturbances to acoustic pressure waves via V-T relaxation processes, with ROTADE the thermal disturbance is detected directly. The excited molecules diffuse in space, come into contact with a receiver such as a QTF, and transfer their energy directly to the receiver. Because the laser induces a periodic excitation of the gas molecules, the QTF undergoes periodic thermal expansion and contraction cycles. The heating of the QTF is converted via the indirect pyroelectric effect [4] to a mechanical stress and then to an electric charge separation which can be measured. In this paper, we describe a general mathematical model for a ROTADE sensor. We also describe a preliminary study to determine the effect that localized heating of a QTF has on the received signal. For this study we applied heat directly to the surface of the QTF rather than using the heat source to detect a trace gas. The goals of the study are to determine the optimal location of the heat source with respect to the QTF and to provide an initial validation of the model.

2. Mathematical model

We use the theory of linear thermoelasticity [5] to develop a two-stage model for the QTF deformation that is induced by a time-harmonic heat source. First, we use the heat equation to model the generation of thermal waves due to the interaction of the laser and the trace gas and the resulting periodic diffusion of heat into the interior of the QTF. Second, we express the mechanical stress, S, produced by the change in temperature, T, via the stress-strain-temperature relation, $S = C[E] - C[\alpha T]$, where E is the total strain tensor (*i.e.* the sum of mechanical and thermal strains), C is the elasticity tensor, and α is the thermal expansion tensor. Consequently, the equation that describes the structural deformation of the tuning fork is

$$\nabla \cdot C[\nabla \mathbf{u}] + \rho\omega^2 \mathbf{u} = \nabla \cdot C[\alpha T],$$

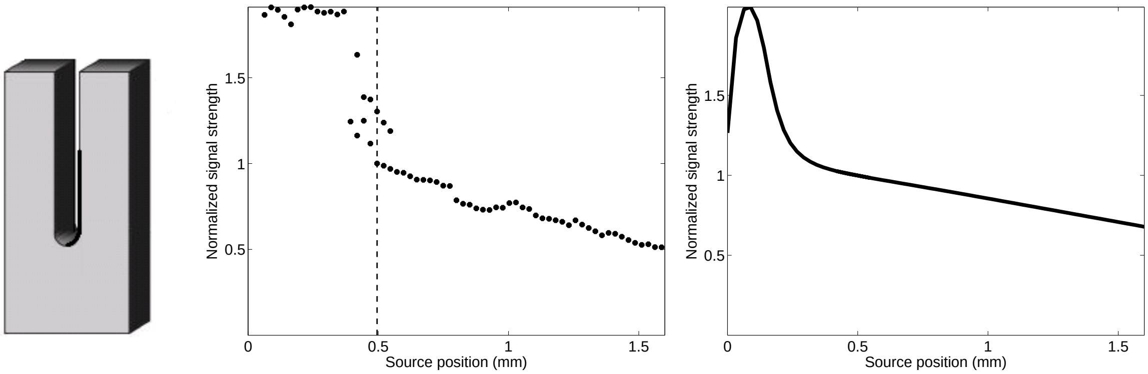

Fig. 1. The QTF with the range of heat source positions used in the simulation shown with a thick solid line (left), and the normalized signal strengths from the experiment (center) and simulation (right).

where ω is the angular frequency of the time-harmonic heat source, which is chosen to be equal to the resonance frequency of the QTF. To match the experimental configuration, the appropriate boundary conditions are constrained displacement on the base of the QTF, and zero traction on the other surfaces [5]. We calculate the received electrical signal from $\mathbf{u}$ as in [6].

3. Experimental and simulation results

A typical ROTADE setup consists of a QTF and a modulated laser beam focused between the tines of the tuning fork. Although the ROTADE sensor will be used to detect trace gases, for this paper we performed a preliminary experiment in which localized heat was directly applied to the QTF using an amplitude-modulated laser. To minimize the possibility of interference due to a QEPAS signal, the experiment was performed in a vacuum. We numerically computed the deformation of the tuning fork due to this localized heating. To focus on the effect of the heat source position, we approximated the temperature distribution in the QTF by a 3D Gaussian with a FWHM of 10 μm. For the experiment, we varied the heat source position along a vertical line located near the inner edge on one of the tines of the QTF. The range of source positions for the simulation is given by the thick solid line in Fig. 1 (left). We positioned the heat source close to the curved surface of the QTF in the simulation so as to obtain a better approximation to the thermal distribution in an actual ROTADE sensor than was possible in the experiment.

In Fig. 1, we plot the experimental signal strength (center) and the numerical signal (right) as functions of the vertical distance of the heat source above the bottom of the ‘U’ of the QTF. There is good agreement between the experiment and simulation to the right of the vertical dotted line in Fig. 1 (center). (To the left of the dotted line the experimental results may be affected by electrodes on the QTF surface.) Both results indicate that the signal is largest when the laser is positioned near the bottom of the ‘U’. By comparison, in [1], [6] we showed that for a QEPAS sensor the laser should be positioned near the top of the QTF. These results will be used in the design of a ROTADE sensor.

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