Theoretical Analysis of a Quartz-Enhanced Photoacoustic Spectroscopy Sensor

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Abstract: A quartz tuning fork interacting with a laser-generated pressure wave can be accurately modeled via a system of coupled partial differential equations. The model predicts the optimal placement of the laser as validated by experiment.

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1. Introduction The current development of mid infrared sensor systems involves combining a quantum cascade laser with a quartz enhanced photoacoustic spectroscopy (QEPAS) technique [1], [2]. These systems will enable trace gas quantification for various applications including urban air quality monitoring, industrial process control, and non-invasive medical diagnostics using breath biomarkers. QEPAS sensors provide high sensitivity, immunity to environmental acoustic noise, and portability with potentially low cost.

In this paper, we describe an analytic model of the QEPAS sensor currently being developed by Kosterev et al. at Rice University [1]. This sensor is based on a novel approach to photoacoustic detection that uses a quartz tuning fork as a resonant acoustic transducer. To detect the presence of a trace gas, a wavelength modulated laser beam is passed between the tines of a tuning fork. When optical radiation is absorbed by the trace gas, the medium undergoes periodic thermal expansion which gives rise to a weak acoustic pressure wave. The pressure wave causes the tines of the tuning fork to vibrate thereby generating an electrical signal via the piezoelectric effect. Prior work modeling tuning fork sensors includes an outline for a qualitative model of the piezoelectric signal generated in a QEPAS sensor [2], and a model based on a vibrating cantilever [3]. In this paper, we present the first quantitative mathematical model of a QEPAS sensor without a microresonator. We use the model to validate the experimentally detected optimal position of the laser beam relative to the tuning fork.

2. Mathematical model The acoustic pressure wave in free space is modeled by the inhomogenous wave equation

$$\frac{\partial^2 P}{\partial t^2} - c^2 \Delta P = S,$$

where t is time, P is pressure, and c is the sound speed. We model the source S as the product of a constant-width radial Gaussian function and a simple harmonic in time, *i.e.* $S = W e^{-\frac{r^2}{2\sigma^2}} e^{i\omega t}$, where r is radial distance from the axis of the beam, ω is the wavelength modulation frequency, σ is the width of the laser beam, and W is determined the laser power and the concentration of the trace gas. Because of the cylindrical symmetry of the beam, the solution depends only on r and t. We derive a pressure wave solution which, when r is large relative to σ, is well approximated by a combination of Bessel functions:

$$P(r,t) \cong \frac{\pi\sigma^2}{2c^2}\left[J_0\left(\frac{\omega r}{c}\right)\sin(\omega t) - Y_0\left(\frac{\omega r}{c}\right)\cos(\omega t)\right].$$

To model the vibration of the tuning fork in response to this acoustic pressure wave, we regard each tine of the tuning fork as a vibrating one-dimensional cantilever. The equation that governs the damped motion of a vibrating beam is the Euler-Bernoulli equation [4]:

$$EI\frac{\partial^4 u}{\partial y^4} + 2\gamma\frac{du}{dt} + \rho A\frac{\partial^2 u}{\partial t^2} = f(y,t).$$

Here y is distance along the axis of a tine of the tuning fork from its base as shown in Fig. 1 (left), and $u(y,t)$ is the displacement at time t of a point at position y. The force density $f(y,t)$ is given by the difference between the pressure at the inner and outer surfaces of the tine multiplied by the thickness of the tine. The parameters of the tine are Young's modulus, E, the moment of inertia, I, the damping coefficient, 2γ, the density of quartz, ρ, and the cross-sectional area, A. The appropriate boundary conditions for a tine of length L are $u(0,t) = 0$, $\frac{\partial u}{\partial y}(0,t) = 0$, $\frac{\partial^2 u}{\partial y^2}(L,t) = 0$ and $\frac{\partial^3 u}{\partial y^3}(L,t) = 0$ [4]. The derivation of the analytic solution of this problem involves using separation of variables to reduce the problem to an eigenproblem. Since the system is forced at the fundamental resonance frequency ω_0 of the tuning fork (*i.e.* we choose $\omega = \omega_0$), we may assume that the signal is determined by the amplitude, B, of the steady state solution corresponding to the fundamental eigenfunction Φ_0, namely

$$B(y) = \frac{1}{\rho A\sqrt{(\omega_0^2 - \omega^2)^2 + (2\gamma\omega)^2}} \frac{|\int_0^L f(y)\Phi_0(y)dy|}{\int_0^L \Phi_0^2(y)dy}\Phi_0(y).$$

Following [3], we assume that the piezoelectric current is proportional to the displacement of the end of the tine of the tuning fork.

3. Results To validate the model we compare it to experimental results obtained using a 32.8 kHz tuning fork with each tine of length $L = 3.8$ mm; other dimensions are given in [1]. The tuning fork parameters are $E = 7.87 \times 10^{10}$ Pa, $I = 6.12 \times 10^{-15}$ m^4, $\rho = 2.6 \times 10^{-3}$ kg/m^3, and $A = 2.04 \times 10^{-7}$ m^2. The damping coefficient is given by $\gamma = \frac{2\pi f_0}{2Q}$ where the measured quality factor is $Q = 14,000$, and the computed value of the fundamental frequency is $f_0 = 36.9$ kHz. The trace gas to be detected was methane. A laser beam of width $\sigma \approx 0.05$ mm was focused between the tines of the tuning fork at a vertical position y_0 on the axis of the fork as shown in Fig. 1 (left).

We compare the theoretical and experimental results by plotting the normalized signal strength as a function of the beam position y_0. In Fig. 1 (right) we compare the measured data (dots) with the solution from our model (solid curve). The theory confirms that the signal is the strongest when the laser beam is focused at $y_0 = 3.2$ mm. In conclusion, our model demonstrates that a 2 mm change in the location of the laser beam along the tuning fork axis can result in a decrease in the signal strength by a factor of 10.

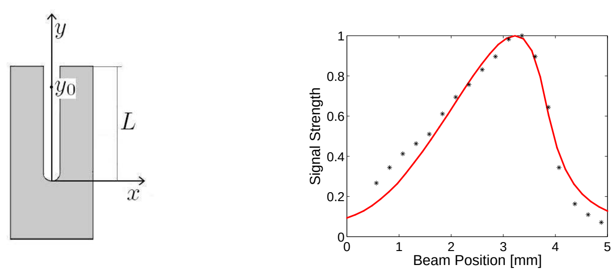

Fig. 1. Left: Diagram of tuning fork. Right: Normalized signal strength versus position y_0 of the laser beam.

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