A Computational Study on Detection of Ultra Small Volumes of Liquid and Solid Media in Microcavities Using Surface Acoustic Wave Devices

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ABSTRACT

In this study, we use finite element method (FEM) analysis to investigate a surface acoustic wave (SAW) based system. This platform involves a regular SAW device with two interdigitated transducers (IDTs) as input and outputs along with a microcavity etched in the middle of the delay line for sensing. This sensing part of the system houses liquids and solid microbeads for the purposes of our simulations. With a peak frequency of 200 MHz, the system mechanically analyzes sample volumes less than 10 pL through coupling of Rayleigh waves to the captured samples. In mixture of glycerin and water between 40% and 90% an approximately linear relation exists between the output phase and glycerin percentage. At this range, a maximum change in the phase of -0.77º was obtained per glycerin percent for microcavities with a depth of 8 µm. When microbeads with a stiffness of 3 GPa are placed in a liquid mixture of 10% glycerin, a linearized sensitivity of -69.4 º/GPa around 3 GPa point is obtained.

Keywords: surface acoustic waves, microcavity, liquid sensing

1 INTRODUCTION

Analysis of relatively small volumes of materials, including liquids and solids has been a topic of interest for various sensing methods and platforms, ranging from atomic force microscopy studies to acoustic waves. Examples of studies include those that investigate the viscosities of solutions [1, 2] as well as those that are aimed towards determining deformabilities of biological samples such as cells and tissues [3, 4]. In order for materials and entities with complex mechanical properties such biological cells to be sensed with adequate resolution and accuracy, a microsystem must be scalable to accommodate such small sizes, provide the required level of sensitivy, and be modeled accurately to reflect the behavior of materials in real life situtations.

In this study, we use FEM analysis to show the possibility of the microsystem shown in Figure 1, is capable of detecting and analyzing liquid and solid media in minute amounts using SAW devices with microcavities. Liquid samples of interest are placed in a microcavity etched into the middle of a delay line with unapodized transducers whereas solid samples are placed inside the liquid solution for enhancing the coupling between piezoelectric and solid domains. Our previous studies on the finite element analysis of the system showed this platform to be viable for use with aqueous solutions [5].

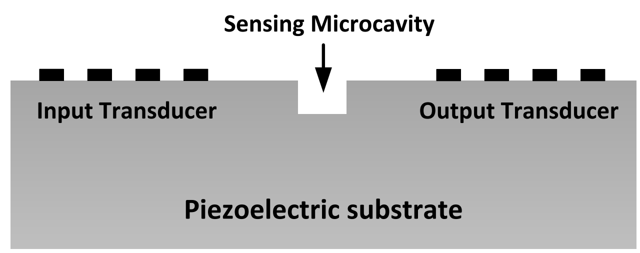

Figure 1: The SAW microcavity system.

2 FEM MODEL OF THE SYSTEM

2.1 Overview

The SAW system includes three separate domains that need to be modeled differently: piezoelectric, liquid, and solid domains (if a solid microbead is placed in the system). The piezoelectric material is defined by its coupling, elasticity, and relative permittivity tensors as well as its density. The material of choice for SAW propagation has been ST-cut quartz (in the x-direction) as it is convenient from a fabrication standpoint to form microcavities and supports Rayleigh waves although it has a low coupling constant as a drawback. The liquid analyte has a certain viscosity, sound velocity, and density as mechanical parameters. One proposed model for viscous liquids is to use a Maxwellian approach and account for viscoelasticity by incorporating a relaxation time given by the ratio of viscosity (η) to its shear modulus (μ). This time constant or relaxation time (τ) shows that the angular operation frequency (ω = 2πf) is an important parameter that must be considered. The magnitude of relaxation time in relation to the angular frequency determines the behavior of the liquid. For $\omega \gg \tau^{-1}$, it behaves closer to a solid whereas for $\omega \ll \tau^{-1}$, it behaves as a Newtonian liquid. For frequencies around 200 MHz that we are considering, estimated shear modulus of glycerin-water mixtures are quite large thus yielding a small time constant. For this reason, a Newtonian liquid model is used. Regarding the polystyrene solid, we employ a standard linear solid model with a stiffness modulus (elasticity and Young's modulus are also used to refer to this parameter), Poisson's ratio, and density. So the mechanical deformations are assumed to take place instantly inside the solid and these deformations are small enough to be considered linear.

2.2 Simulation Model

The system has a harmonic time dependence which makes it convenient to be simulated using a frequency domain solver. Due to the symmetry in the out of plane direction, the system is modeled in two dimensions which also allows for more rapid data collection. Perfectly matched layers (PMLs) are used on the bottom and sides of the model to effectively attenuate the outgoing SAWs from the system and avoid reflections. The meshes for both the liquid and solid sensing models contain approximately 25,000 elements with the normalized element quality histogram as shown in Figure 2. Elements are generated more densely closer to the surface with smaller elements to improve accuracy as shown in Figure 3.

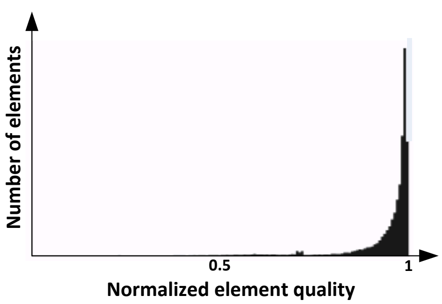

Figure 2: Element quality histogram showing a high mean element quality over all domains.

The wavelength of the Rayleigh type SAW is 16 μm with 64 pairs of unapodized electrodes having a metallization ratio of unity on each side of the microcavity. The microcavity depth varies with some of the simulations but the width is always set to 24 μm which was seen to provide a high sensitivity in simulations not presented here. The thickness of the system in the out-of-plane direction is 24 μm. In all cases, the total volume of the microcavity is smaller than 10 pL. The substrate is modeled to be 40 μm high, and appropriate boundary conditions are applied to minimize reflections from the bottom of the substrate. At the top of the liquid region, a soft boundary is applied to reflect the waves back into the domain while keeping the phase constant. Boundary load and normal acceleration conditions are applied to simulate the coupling of liquid to solid and liquid to piezoelectric layers, and vice versa. It should also be noted that all interfaces with liquid are assumed to have no slip.

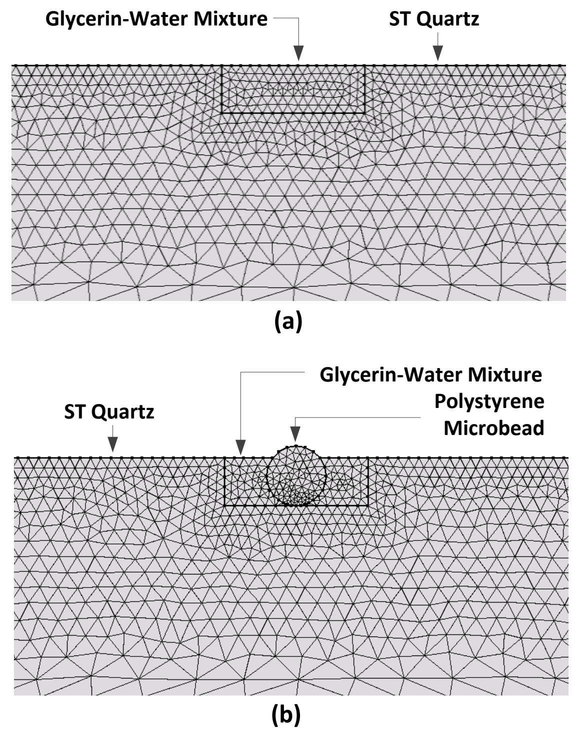

Figure 3: Meshes for (a) liquid and (b) solid sensing modes.

3 SIMULATION RESULTS

It is well known that liquids couple strongly to Rayleigh type surface waves due to the component of displacement directed into the liquid. In our case, Rayleigh waves traveling along the edges of the microcavity region have a boundary with the liquid sample and the transverse component of these waves cause ultrasound waves to be emitted into the liquid. This actuation works both ways and a short while after the initial application of electrical signal to the input IDT, a resonant cavity condition is achieved inside the microcavity.

The primary differences between the liquid and solid loads arise due to the properties of waves that are coupled to these two media. Phase changes are introduced into the output signal based on the acoustic properties of the liquid which enables the determination of mixture content for the liquid case. Although a similar argument to liquids can be made for the solids case, solids support shear waves bringing the elasticity modulus, density, and Poisson's ratio parameters into the equation. For the microbeads, the elastic modulus is varied to observe phase changes. It should be noted that in either case, the system operation contrasts with the conventional mass loading delay lines based on the simulations that show the frequency shifts and magnitude drops are not proportional to mass.

3.1 Liquid Sensing

Glycerin-water mixtures are adopted as the standard liquid for simulations due to their widely accepted acoustic parameters. Table 1 provides an overview of the properties of the liquids used for simulations [6,7].

Glycerin by volume (%)	Glycerin by mass (%)	Density (kg/m^3)	Sound speed (m/s)	Viscosity (mPa·s)
40	45.8	1118	1719	4.3
50	55.9	1145	1733	7.4
60	65.5	1171	1763	14.0
70	74.7	1195	1795	30.0
80	83.5	1218	1817	75.7
90	91.92	1241	1869	241.7

Table 1. Properties of glycerin mixtures in water.

For the given values of liquid parameters, the system is simulated and the output phase is calculated in each case at the peak frequency of the SAW filter. Figure 4 shows the resonance conditions inside the microcavity and the results in terms of phase is given in Figure 5.

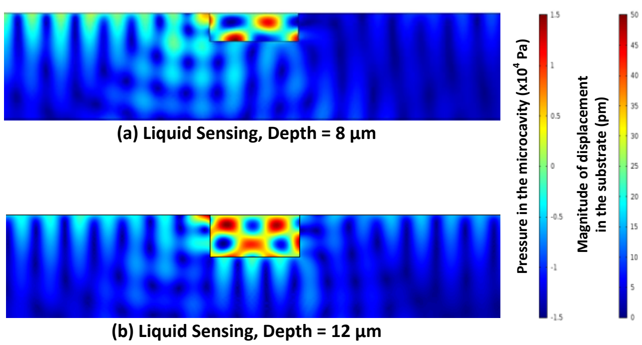

Figure 4. The resonance inside microcavities for two difference microcavity depths. The color maps identify the pressure inside the liquid and displacement inside the piezoelectric domain.

The dependence of the magnitude of insertion loss on liquid properties is limited by the bulk wave conversion that occurs due to the surface irregularity introduced by the microcavity. The frequency shifts in the output are usually associated with mass loading of a resonating crystal. Strong direct correlations between peak frequency shift and liquid properties are only observed for very shallow microcavities. This behavior shows microcavity operation converges to that of a standard delay line at depth of zero as expected [5]. The maximum sensitivity achieved is -0.77 °/percent glycerin with a microcavity depth of 8 µm.

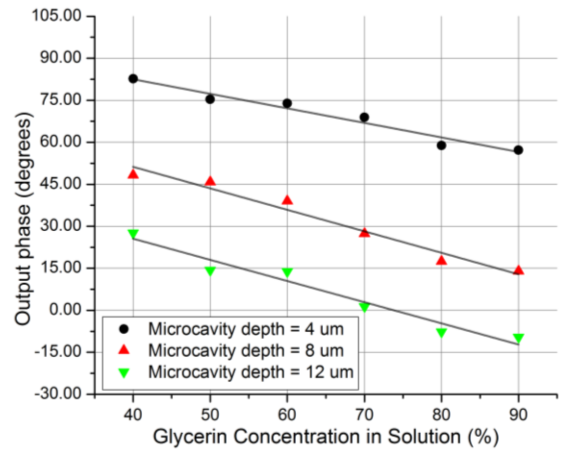

Figure 5. Output phase as a function of glycerin concentration in mixtures in the microcavity.

3.2 Solid Sensing

As mentioned previously, piezoelectric to liquid coupling is usually a very effective mechanism given the properties of most of the common liquids. For solids, the acoustic impedance can vary by a large amount which can render some measurement ranges unusable for the sensor configuration at hand. For this reason, a pressure transmission study was conducted to obtain the effect of stiffness and Poisson's ratio at 200 MHz as shown in Figure 6. Given a density similar to that of water, pressure transmission from the quartz piezoelectric domain to the solid begins only around 10 MPa and has a relatively larger slope with respect to stiffness after roughly 1 GPa. The results show that in the low elastic modulus region, the reflection from the solid material is too high, meaning that interaction with the sample would be severely hampered for the current design.

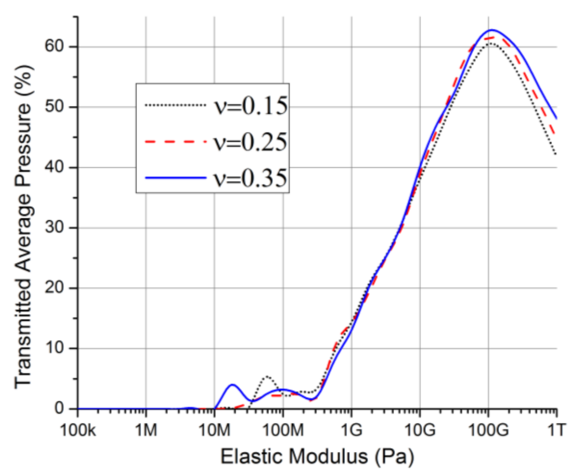

Figure 6. Pressure transmission into solid domain for varying stiffness (or elastic modulus) values at 200 MHz. The density of the solid domain is set to 1000 kg/m^3.

To test the system response to sensing and differentiating between solids, the method of application should first be identified. In order to be able to measure different samples with a given sensor and make the SAW sensor reusable for future tests, the sample should be removable from the microcavity easily. A natural choice at this point is polystyrene microbeads as they are convenient to apply with properties listed in Table 2.

Density (kg/m^3)	1050
Elastic Modulus (GPa)	2.9 – 3.6
Poisson’s Ratio	0.35

Table 2. Properties of polystyrene microbeads.

Polystyrene microbeads come are in a spherical shape not perfectly conforming to the liquid domain. In order not to limit the interaction surface between the substrate and microbeads, the 10 µm diameter microbeads have been placed in a liquid with known properties, a 10% glycerin-water mixture. The liquid acts as a coupling medium and provides transmission of the SAWs as shown in Figure 7.

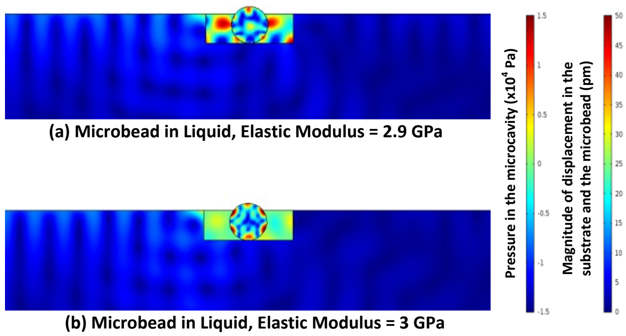

Figure 7. Microbeads in liquid with the resonance patterns shown in the color map. The liquid used is 10% glycerin in water and microcavity depth is 8 µm.

Despite the irregular shape of the bead, results in Figure 8 show that bead elastic modulus can be indirectly measured using this method. A linear fit on the transfer curve for output phase provides a sensitivity of -69.4 °/GPa.

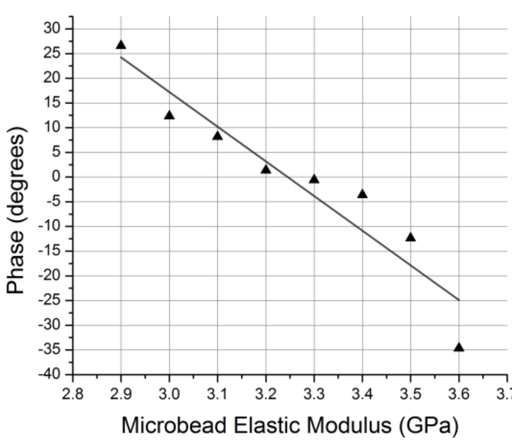

Figure 8. Stiffness of the polystyrene microbead versus the system phase angle.

4 CONCLUSION

In this study we presented a SAW system that exploits the generally unwanted strong liquid coupling nature of Rayleigh waves to be used as a sensor through addition of microcavities. The system was modeled and simulated using FEM analysis tools. In mixtures of glycerin and water between 40% and 90% a roughly linear and reasonable relation exists for velocity of sound and density, and at this range, a maximum phase change of -0.77 º/glycerin percent for 8 µm deep microcavities. Following this result, when the microbead is added to the system, a further decrease is obtained in the phase for microcavity of the same depth. The higher non-linearity of the results in the microbead case is due to the irregular spherical shape of the microbead inside the rectangular microcavity that makes the results harder to read, however a linear fit provides a sensitivity of -69.4 º/GPa around 3 GPa point. On the other hand, simulations also show that the elastic materials to be sensed by the system need to have elastic moduli in the order of GPa’s. Otherwise, the designs need to be modified accordingly or materials closely following the behavior of a different mechanic model should be used.

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