

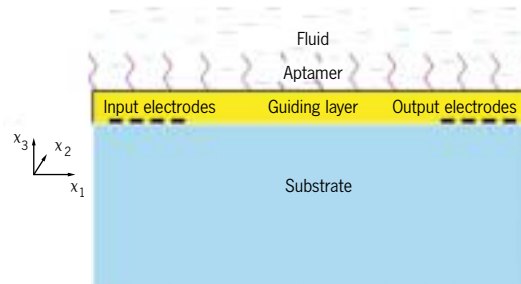
The group 'Modeling' supports the development of a surface acoustic wave sensor (biosensor) based on the generation and detection of horizontally polarized shear waves. Such waves can be excited using a multi-layered structure consisting of a piezoelectric quartz substrate covered by a thin isotropic guiding layer. If the velocity of shear waves in the guiding layer is lower than in the substrate, shear waves will be transmitted into the guiding layer. The guiding layer contacts a liquid containing a ligand to be detected. The ligand adheres to a specific receptor (aptamer) immobilized on the surface of the guiding layer. The arising mass loading yields a phase shift of the shear waves measured by an electric circuit. Our previous work concentrated on the development of mathematical models of the biosensor and their numerical implementation using finite element methods. Because of a quite small wavelength, finite element models require very fine grids, and thus very large computational resources. Therefore, we use a reduction of 3D-models either to front-face models where the averaging in x_2 -direction is done or to a top-face model obtained by the averaging in x_3 -direction under assumptions about the exponential attenuation of wave amplitudes with depth.

Such simplified models are used for the computation of the sensitivity and optimal operating frequency of the biosensor. The results obtained are consistent with physical experiments. However, these models are still very expensive in terms of computational time and resources so that numerous series of computer experiments, where geometrical and material parameters are being varied, can hardly be performed.

A way to speed up numerical simulations consists in the usage of dispersion relations which express the dependence of the surface shear wave velocity on the operating frequency. Many characteristics of the biosensor can be computed on the base of dispersion relations. The derivation of dispersion relations is a complicated problem that is solved nowadays for simple structures consisting of few isotropic solid layers.

We proposed a semi-analytic method that solves the problem above for multi-layered structures similar to that in Fig. 1. Thereby, each of the solid layers can be anisotropic and the number of solid layers is not restricted. A fluid and a bristle layer (aptamer) on the top of the upper solid layer are accounted for.

Figure 1: A draft of a front cross-section of the biosensor. Acoustic shear waves are excited by the left electrodes deposited on a quartz crystal substrate. The waves propagate to the right and are detected by the right electrodes. To obtain purely shear-polarized modes, the direction of the wave propagation is chosen to be Y-crystallographic axis of the quartz crystal. A guiding layer is necessary to obtain surface shear waves. An aptamer absorbs desired bio-molecules from a liquid.



Cross-links:

Aptamer Biosensor

Development of
Microbalance Array/
Mass Spectrometry

Biomechanical Modeling

Cooperations:

University of Bonn

The method is based on the consideration of a plane wave propagating in x_1 -direction. The wave satisfies elasticity equations in every solid layer and linearized Navier-Stokes equations in the fluid. The dispersion relations are computed from the continuity of displacements and normal pressures on the interfaces between the solid layers, continuity of velocities and pressures on the solid-liquid interface, and the exponential attenuation of the wave amplitude in the substrate. The aptamer layer is accounted for by the calculation of the averaged horizontal force produced by the liquid, which results in some modification of the normal pressure continuity condition on the solid-liquid interface. Numerically, the problem is reduced to the statement and solution of a system of transcendental equations whose roots represent propagating velocities for different wave types. As a rule, there are three roots corresponding to transversal, shear, and longitudinal surface acoustic waves, respectively. A computer program that implements the computation of the wave propagation velocity depending on the operating frequency is very effective. It allows us to compute very interesting dependencies presented in Figs. 2–4 within several seconds.

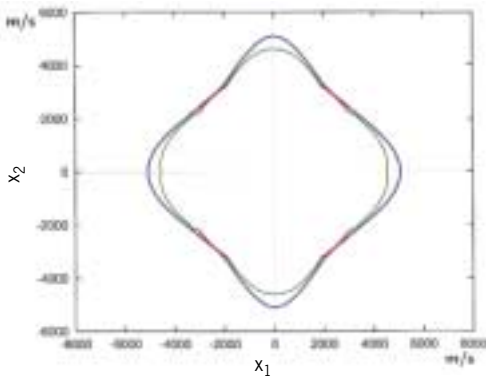


Figure 2: Velocity diagram for an operating frequency of 112.2 MHz. The green line corresponds to a substrate-guiding layer structure. The blue line shows the velocity of bulk waves in the substrate.

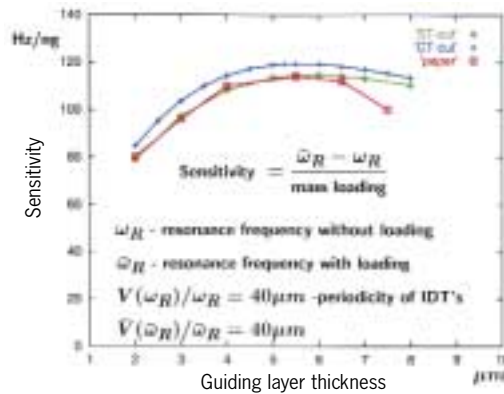


Figure 3: Dispersion relations allow us to estimate a sensitivity of the biosensor. The results are compared with: G.L. Harding, Mass sensitivity of Love-mode acoustic sensors incorporating silicon dioxide and silicon-oxy-fluoride guiding layers, Sensors and Actuators A 88 (2001).

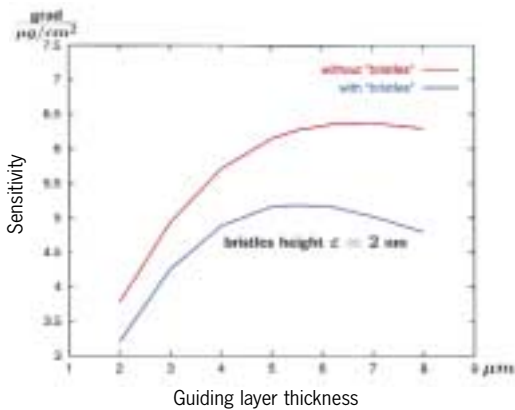


Figure 4: This is another sensitivity characteristic computed using dispersion relations in the presence of a liquid and a bristle layer modeling an aptamer. The simulation shows that even a very thin aptamer layer affects the sensitivity.