Mathematical modeling of a biosensor

Biosensors serve for measuring small amounts of biological substances in gaseous and liquid environments. Love-mode acoustic devices based on the generation and detection of horizontally polarized shear waves are especially suitable for sensing in liquids. Acoustic shear waves are excited due to an alternate voltage applied to input electrodes deposited on a piezoelectric substrate covered by a thin isotropic guiding layer. If the velocity of shear waves in the guiding layer is less than the one in the substrate, shear waves are transmitted into the guiding layer. The guiding layer contacts a liquid containing biomolecules to be detected. Biomolecules adhere to a specific receptor, aptamer, immobilized on the top of the guiding layer. The arising mass loading causes a phase shift in the electric signal to be measured by output electrodes.

Mathematical model

\[ \rho \ddot{u} - \nabla \cdot \sigma = - \nabla \cdot \left( \mu \nabla \dot{u} - \frac{\zeta}{\eta} \frac{\partial \dot{u}}{\partial t} \right) \]

FE-Simulations for a reduced 2D-model

Usage of dispersion relations

Dispersion relations express the dependence of the shear wave velocity on the operating frequency. We compute dispersion relations for multi-layered anisotropic structures like the biosensor. This enables us to calculate the phase shift of waves depending on the mass loading. Figures to the right present measured and computed phase shift in the real time process of copper etching by an acid.

Modeling of biomolecular layers using homogenization

A very important issue in the simulation of the biosensor is modeling of aptamers and adhering biomolecules on the sensor’s surface. One can consider the aptamer (biomolecular) layer as a periodic bristle structure contacting the liquid. The bristle-fluid structure is replaced by an averaged material whose properties are being derived as the number of the bristles goes to infinity whereas their thickness goes to zero. The height of the bristles is assumed to be constant.

The limiting equation describing the averaged material:

\[ \rho u_{tt} - \nabla \cdot (\mu \nabla u) - \nabla \cdot (\eta \dot{u}) - \nabla \cdot \left( \frac{\zeta}{\eta} \frac{\partial \dot{u}}{\partial t} \right) = 0 \]

Using a homogenization technique, extremely high sensitivities of the sensor measured in experiments through adhering biomolecules can be explained. It happens because biomolecules take the liquid boundary layer completely along. We model this effect by choosing appropriate parameters of homogenization. The picture to the right shows the computed phase shift for a multi-layered structure consisting of a quartz substrate, an SiO$_2$ guiding layer, a gold shielding film, aptamer and protein layers.

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