Biosensors combine the high selectivity and sensitivity of molecular recognition processes of biological macromolecules with a transducer. The increase in mass by the recognition process can in principle be detected by a mass sensitive transducer, which converts the result of the recognition event into an electrical signal. High sensitivity of the transducer regarding mass loading is needed in order to detect the molecular recognition process. Mathematical modeling of the transducer is used to optimize the parameters with respect to the sensitivity. Fig. 1 shows the schematics of the biosensor.

The mathematical model represents a composite structure consisting of three coupled layers: two solid layers with different elastic and electric properties and a liquid layer treated as a compressible viscous fluid. Full coupling between deformations and the electric field is assumed. The model takes into account the massiveness of the electrodes and the influence of acoustic absorbers, which reduce the reflection of waves at the ends of the device. The model is realized on the basis of finite elements and uses automatic derivation of the model equations for various crystal cuts.

Fig. 2 shows the steady-state solution of the shear waves in the different layers computed using a reduced 2D model in the $x_1,x_3$ plane. The computation is performed for crystalline quartz substrate and a SiO$_2$ layer for three designs of electrodes, the operating frequency is 81 MHz and the periodicity of electrode lines is 40µm. The results show good wave propagation within the guiding layer and strong attenuation of shear waves in the substrate. The penetration depth of shear waves into the fluid is in the range of one wavelength.

Figure 1: Acoustic shear waves are excited due to an alternate voltage applied to microstructured thin film electrodes deposited on a quartz crystal substrate; the waves are transmitted into a thin isotropic guiding layer which is in contact with a liquid containing the molecules to be detected; this ligand adheres to a specific receptor immobilized on the surface of the guiding layer; the mass loading causes a phase shift in the electric signal which is measured by the sensor. To obtain purely shear-polarized modes, the direction of the wave propagation is chosen to be orthogonal to the crystal's x-axis. The choice of the film and substrate materials must ensure that the wave velocity in the film is less than the one in the substrate. The mathematical model helps to design the biosensor with respect to the thickness of the layer, the position of the interdigital transducers (IDTs) and the frequency and amplitude of the acoustic shear waves.

Figure 2: a) $x_2$-velocity in the fluid, b) shear waves in the guiding layer, c) shear waves in the substrate.
The simulations are used to obtain the frequency where damping of the signal is minimized. In order to specify this frequency the number of electrode lines in the sensor is increased. Simulation for a real sensor with 50 pairs of input and output electrodes using a reduced model in the \(x_1,x_2\) plane are shown in Fig. 3. The optimal operating frequency obtained with these simulations is 130 MHz.

The computed values of the resonance frequencies are in a good agreement with the values obtained from measurements.

Variations in the thickness of the guiding layer show the high sensitivity of the model with respect to small mass loadings. With the help of this simulations time consuming experiments can be reduced. Especially a thickness of the guiding layer above 8 µm can be excluded for further considerations due to the simulation results, favoring a thickness in the range of 5.5 µm to 7.5 µm. The model will be used for further design optimization of the biosensor.

Besides the use in biosensors the model can be applied in the development of other sensors where wave propagation is concerned.