

Cross-links:

MAMS: Aptamer Biosensors

MAMS: Mass Spectrometry and Bioinformatics

The investigation of dispersion relations is motivated by the modeling of a biosensor that serves for the detection and quantitative measurement of small amounts of biological substances. The operating principle of the biosensor is based on the generation and detection of horizontally polarized shear Love waves. From the mechanical point of view, the biosensor is a multi-layered structure consisting both of isotropic and anisotropic layers (see Fig. 1). A biological substance adheres to the surface of the top layer so that a new layer is being formed, which changes the velocity of shear waves propagating along the sensor surface. Thus, an effective tool for computing the velocity of waves in multi-

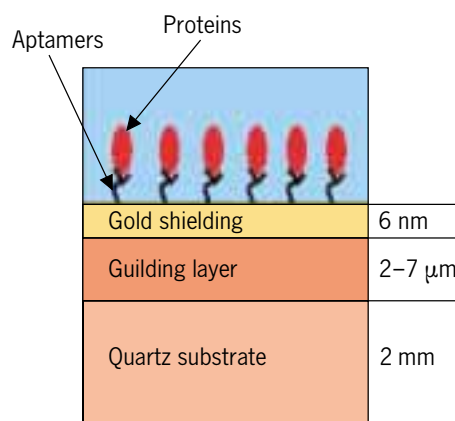


Figure 1: Cross-section of the biosensor structure.

layered structures would enable us to estimate the sensitivity of the biosensor in dependence on its constructive features and operation parameters.

Classical examples of the derivation of dispersion relations demonstrate that the problem is solvable analytically in simplest cases only. Therefore, it is reasonable to examine semi-analytical methods that use both analytical representations of solutions and numerical determination of their parameters. Such a method and the related program are developed by the authors.

The algorithm is based on the construction of traveling wave solutions of elasticity equations describing deformations in the layers. The wave velocity is computed from the fitting of mechanical conditions on the interfaces between the layers. These conditions express the continuity of the displacement field and the pressure equilibrium for each pair of the layers. Feasible wave velocities are the roots of a non-negative real function (fitting function) that expresses a measure of the inconsistency in the interface conditions. Comparing with other existing developments our program is especially effective for very thin layers. The program is supplied with a user friendly graphical interface written in Visual C++. Using this interface, one can compose a multi-layered structure consisting of arbitrary number of isotropic and anisotropic layers. The material properties such as elastic stiffness tensors can easily be set and edited. If a layer is anisotropic, the orientation of its material is described in terms of successive rotations of the reference system. It is possible to import material parameters from existing models, which is especially convenient when dealing with elastic stiffness tensors that contain a lot of coefficients. After composing the structure and specifying the wave frequency, the fitting function is computed and graphically presented (see Fig. 2). Now, the roots of the fitting function can be localized and found precisely along with polarization vectors that indicate the wave types. Moreover, the program possesses an option for the automatic computation of dispersion curves (dependencies between the wave velocity and the frequency) for given frequency intervals. Such features make the program useful for researchers working on acoustic sensors.

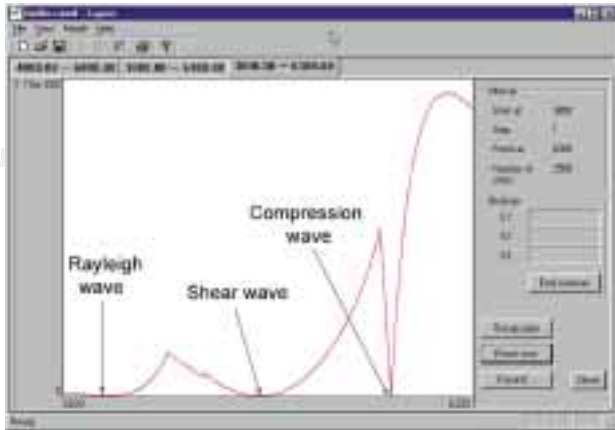


Figure 2: The main window of the program. Roots of the fitting function are the wave velocities for different wave types.

A procedure for describing the propagation of surface acoustic waves in anisotropic-multi-layered structures based on solving Hamilton-Jacobi equations is developed. The computation yields contours of the constant propagation time. The Hamiltonians of the equations are being computed numerically on the base of velocity profiles determined using dispersion relations. Generally, the Hamiltonians are non convex in impulse variables, which leads to the intersection of characteristics when solving such Hamilton-Jacobi equations. Numerical methods of differential game theory are appropriate for solving problems with non convex Hamiltonians. They were applied to the simulation of the biosensor. Fig. 4 shows an example of the propagation of shear surface acoustic waves in a two-layered structure consisting of a quartz substrate and a SiO_2 -guiding layer.

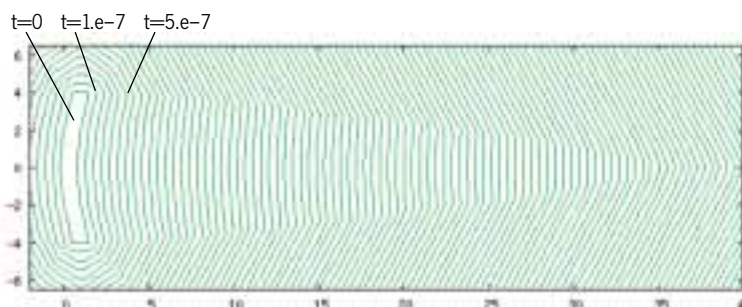


Figure 4: Propagation of shear surface acoustic waves from a curved source.

Fig. 3 demonstrates the application of our method to the verification of physical experiments related to a biosensor developed at caesar. A 9 nm copper film is deposited on the top layer of the biosensor. Curve (a) shows the time performance of the etching of the copper film. The water flux is being alternated with the flux of an acid solution. The phase shift is being measured. Curve (b) represents the phase shift computed using dispersion relations. The simulation proves the assumption that the jump at the acid-to-water transition is caused by the change of the fluid viscosity.

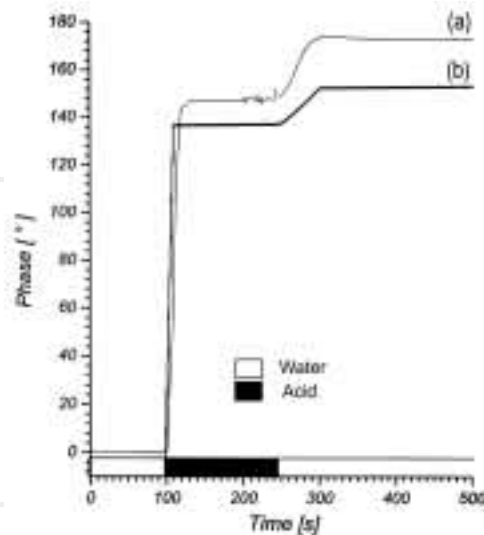


Figure 3: Comparison of numerical simulation with physical experiment: (a) experiment, (b) simulation.

Cooperation:

Institute of Applied Mathematics, University of Bonn

Institute for Problems in Mechanics, Moscow

Institute of Mathematics and Mechanics, Ekaterinburg