MAMS: Mathematical Modeling of a Biosensor

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Cross-links:

MAMS:
Aptamer Biosensors

MAMS:
Mass Spectrometry
and Bioinformatics

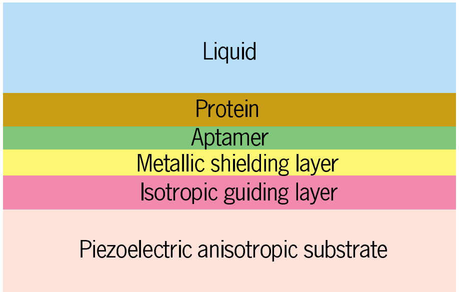
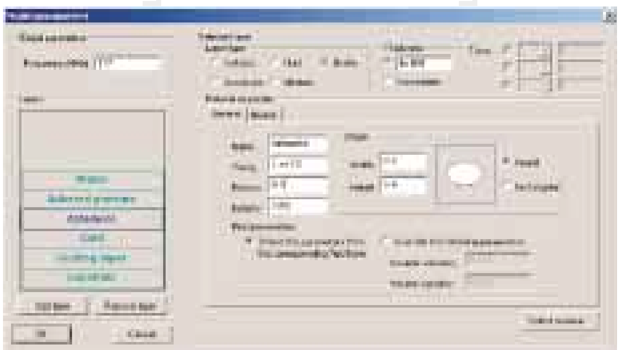


Figure 1: Multi-layered structure typical for biosensors.

Designing diverse acoustic systems and, in particular, biosensors developed at caesar is impossible without the analysis of the propagation of acoustic waves in multi-layered anisotropic structures. An example of the structure typical for biosensoric applications is shown in Fig. 1. The group Modeling is working on a computer program to be applied in biosensorics. The program calculates the velocity of acoustic waves of diverse types depending on the excitation frequency for complex structures typical for bio-sensors. In comparison with a preliminary version, the current one takes into account not only mechanical but also electrical and piezoelectrical properties of materials forming the multi-layered structure under investigation. It is also possible to simulate bristle-like layers which are being formed when proteins solved in a liquid adhere to tiny receptors (apta-mers) immobilized on the surface of the biosensor. The interaction of the structure with such environments as vacuum, gases, and fluids is included in the mathematical model adequately.

Taking into account electrical and piezoelectrical properties of materials, the electrical potential is added to the set of variables of governing equations. The jump conditions of the electric field and the dielectric displacement complete other matching conditions holding at the interfaces between the layers. The accounting for bristle-like structures is based on results obtained using homogenization techniques. The main point of this method is to replace a bristle-fluid layer by an averaged homogeneous layer whose material properties are derived as the number of bristles goes to infinity whereas their thickness goes to zero, thereby the height of the bristles remains constant. The homogenized layer is governed by limiting equations whose tensor coefficients are determined by the parameters of the liquid and solid parts as well as by the geometry of the bristles.



The computation of these coefficients is not trivial: it is based on operator theory and involves finite element methods. Thus, a finite-element module is integrated in the program.

Figure 2: Arrangement of a biosensor-like structure.

Keywords: biosensor, multi-layered structure, dispersion relations

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Figure 3: Profiles of the displacements. Only the displacement orthogonal to the wave vector is different from zero (shear wave).

The program is supplied with a standard windows interface providing convenient tools for operations with parameters of the model (see Fig. 2), which is of great importance since some of the materials are described by various parameters (up to 46 parameters for piezoelectric anisotropic materials). The model can contain an arbitrary number of layers of diverse types: solids (with or without dielectric, piezoelectric, and metallic properties), liquids, enviroment media (vacuum, gas, liquid) and bristle-like structures.

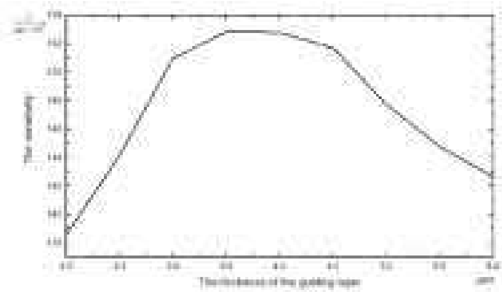

Figure 4: Simulated dependence of the sensitivity of a Love wave sensor on the thickness of the guiding layer.

After determining the wave velocity the user can have a look at the profiles of mechanical displacements and the electric potential inside the layers (see Fig. 3), which delivers very important information about the type of the acoustic wave for which the velocity is found.

The program allows us to compute important dependences such as the sensitivity of biosensors with respect to the thickness of the guiding layer (see Fig. 4), the influence of shielding metallic layers on the velocity of waves, dispersion curves, etc.

The slowness and wave contours for surface acoustic waves can be constructed using the program proposed. Therefore, the Hamilton-Jacobi techniques can be applied to describe the dynamics of the wave phase. Such an approach enables us to find singular characteristics of the eikonal equation which represent the energy flow (the rays). This information can be useful for the study of focusing and beam-steering properties in specially designed transducers. Fig. 5 shows the wave fronts (green) and the singular characteristics (blue, cyan, and red) excited in a biosensor-like structure by a curvilinear transducer.

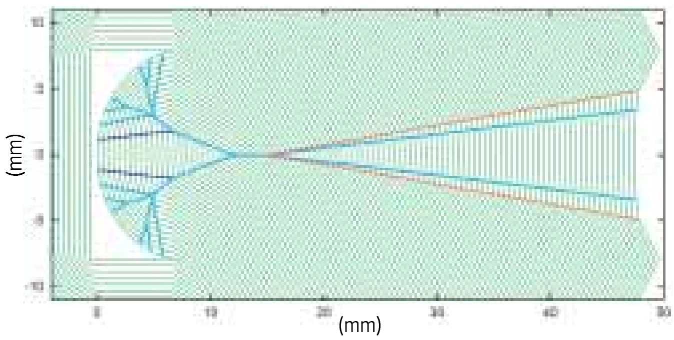

Figure 5: Wave fronts and singular characteristics in a biosensor-like structure.

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Reference: Botkin N.D.; Hoffmann K.-H.; Pykhteev O.A.; Turova V.L.: Dispersion relations for acoustic waves in heterogeneous multi-layered structures contacting with fluids. In: Proceedings of the First International Conference on Modeling, Simulation and Applied Optimization, Sharjah, U.A.E, February 1–3, 2005.