Simulation of Field-Effect Biosensors (BioFETs) for Biotin-Streptavidin Complexes

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Detection of pathogens, tumor markers, and antigen-antibody complexes is an expensive, time consuming, and complex task. Typical steps for detecting a certain DNA strand consist of increasing the DNA concentration by PCR (polymerase chain reaction) or RT (reverse transcription), labeling of the molecule, and applying it to a microarray. Then the microarray is read out in an optical procedure using laser beams. Making optical detection superfluous by an electrical signal has several advantages. Using BioFETs (biologically sensitive field-effect transistors) also makes it possible to integrate additional circuits for amplifying and analyzing the signal on the chip. Therefore BioFET microarrays safe time, space, and equipment, enabling their use outdoors to control the spread of diseases and environmental pollution, without the need of a lab [1].

The components of a BioFET are a semiconductor transducer, a dielectric layer, a functionalized surface with immobilized biomolecule receptors where the analyte binds, and an electrolyte with an electrode. When analyte molecules bind to the receptors, their charges change the potential near the transducer-surface and thus the conductance of the field-effect transistor channel. The change of the potential happens at the Angstrom length-scale, while the device dimensions are on the micrometer length-scale. Therefore it is essential to have an appropriate model to describes the transducer-solution interface.

A homogenized interface model [2] is studied on a common nMOS device to show the generality of the modeling approach for biomolecular detection. For this simulation a biotin-streptavidin complex was chosen because of their use in purification and detection of various biomolecules. The strong streptavidin-biotin binding can also be used to attach various biomolecules to one another or onto a solid support. The charges of the biomolecules were modeled using a bottom-up approach [3] and the charge and dipole moment of a single molecule from the protein data bank [4] is calculated. These values are related to a surface density by choosing the mean distance between the molecules. The connection between the surface silicon oxide and the aqueous solution is realized by two homogenized interface conditions.

The first condition describes the jump in the field, while the second introduces a dipole moment that causes a shift of the potential which is taken into account by adjusting the potential in the solute. The model shows a strong dependence on surface charges and indicates a small shift in the threshold voltage depending on their orientation related to the surface. The bound state (biotin-streptavidin) is

negatively charged with 18.46 elementary charges compared to the unbound state (biotin only) negatively charged with 1 elementary charge. This leads to a reduced conductivity after binding. Also the shift of the threshold voltage and output characteristics due to different molecule orientations (0 degrees - perpendicular to surface, 90 degrees - lying flat on surface) have been calculated.

References

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