

# Numerical Aspects of the Three-Dimensional Feature-Scale Simulation of Silicon-Nanowire Field-Effect Sensors for DNA Detection

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## INTRODUCTION AND MOTIVATION

In recent months experimental silicon-nanowire field-effect biosensors were built and their functioning was verified [1], [2]. These devices consist of a silicon-nanowire core, an enveloping silicon-oxide, and a surface receptor molecule (cf. Fig. 1). When a biomolecule attaches to the surface receptor and this attachment results in a sufficiently different charge distribution, the change in current flow through the nanowire enables detection.

These sensors provide perfect selectivity since the possibility of a binding being established between two biomolecules (a protein and an antibody, for example) is equivalent to having a biological function. Furthermore extremely high detection sensitivity in the pg/ml regime has been reported [1]. It seems feasible that these devices can sense a huge array of biomolecules, and notable application areas are the detection of cancer markers and DNA fragments.

## SIMULATION METHOD

In this work we investigate the numerical aspects and challenges of three-dimensional feature-scale simulations at the example of three states of a nanoscale DNA sensor in aqueous solution. In the first state nothing is attached, in the second state one chain of the DNA fragment (5'-D(CGTGAATTCACG)-3') is attached, and in the third state the whole dodecamer is attached (see Fig. 1, Fig. 2, Fig. 3).

After determining the partial charges on the DNA fragment, their distribution was used to obtain the electrostatic potential by solving the 3D Poisson equation. Charge transport was simulated using a 3D self-consistent NEGF simulator [3].

## RESULTS AND CONCLUSIONS

Simulator timings are shown in Fig. 4, the current-voltage characteristics in Fig. 5, and the potential in Fig. 6. The characteristics imply that the differences in current between the three states allow to discern if a functional device was produced (i.e., a single-stranded fragment is attached) and if a second strand is attached to the first.

The simulations show that the length of the linker is a critical device parameter. The detection of larger and only moderately charged molecules will be correspondingly more difficult.

The calculation of the electrostatic potential around the molecules and in the nanowire necessitates the use of sparse-matrix representations and algorithms to achieve good resolution within modest memory requirements. Transport simulations using the NEGF formalism benefit from parallelization.

(Readers will be able to run simulations on various structures online at <http://www.nanohub.org>.)

## ACKNOWLEDGMENT

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## REFERENCES

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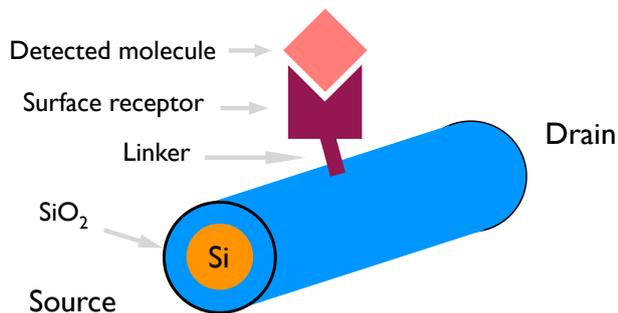


Fig. 1. The structure of a silicon nanowire biosensor. In the simulations the length of the wire is 10nm with a doped region of 4nm in the middle. The diameters of the silicon core and the outer oxide cylinder are 3nm and 5nm, respectively.

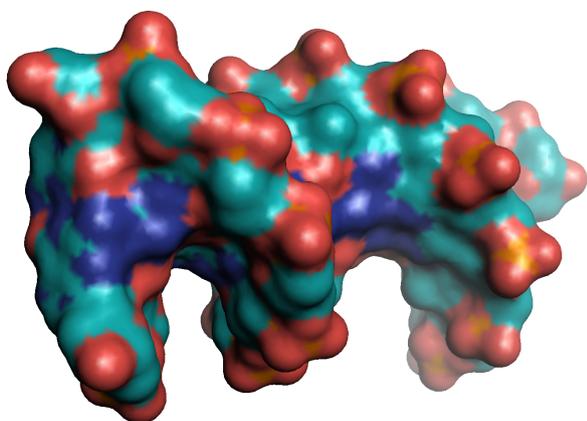


Fig. 2. The double-stranded dodecamer (5'-D(CGTGAATTCACG)-3'). It carries a total of  $-41.74$  positron charges. Its size is approximately  $2\text{nm} \times 2\text{nm} \times 4\text{nm}$ .

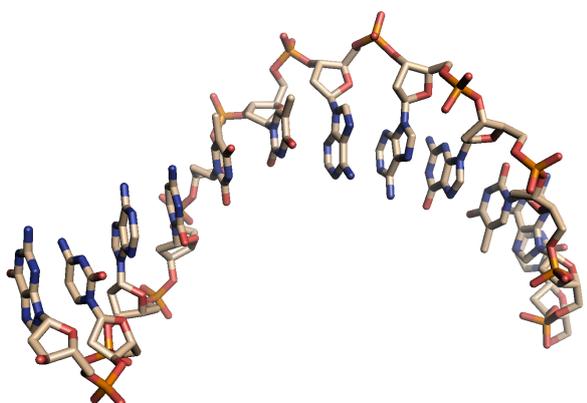


Fig. 3. Chain A of the structure shown in Fig. 2 only. It carries half as many charges, namely  $-20.87$  positron charges.

Schrödinger equation	2.5s
Charge transport (NEGF)	40s
Poisson equation	4.0s

Fig. 4. This table shows the duration of the three parts of the self-consistent loop of the charge transport simulations. A grid spacing of 0.2nm was used in the transport direction which gives 51 slices for the device length of 10nm. The Schrödinger equation was solved for each slice in parallel on 51 processors. In the directions normal to charge transport a grid with 562 nodes, 1611 edges, and 1050 elements was used. In total 28 100 nodes were used for the 3D Poisson solution.

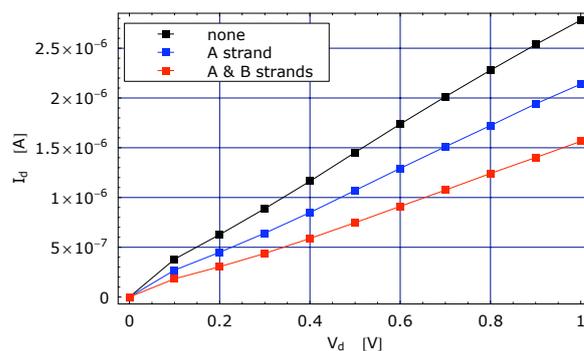


Fig. 5. The current-voltage characteristics for source-drain voltages from 0.0V to 1.0V. The upper most curve corresponds to no molecule attached, the middle curve to single-stranded DNA, and the lower most curve to double-stranded DNA. The addition of each set of charged molecules reduces the current by  $\approx 25\%$ .

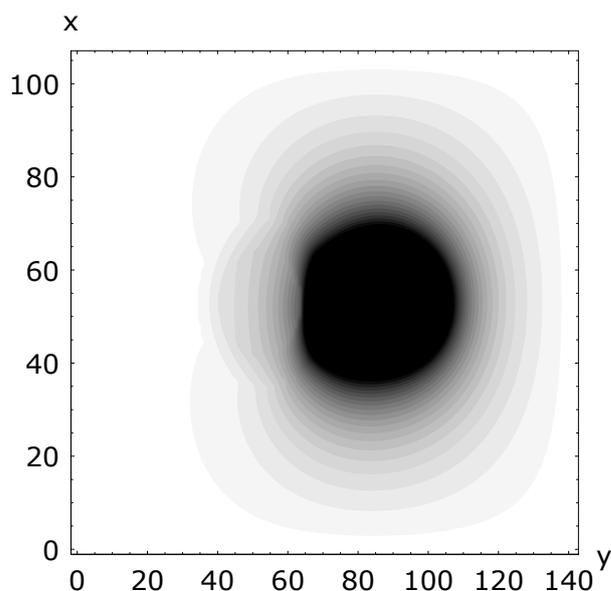


Fig. 6. The potential in a plane normal to the nanowire through the middle of the double-stranded DNA fragment. The shape of the nanowire can be recognized in the left part of the picture.