Analysis of 1D and 3D Distribution of Electric Potential in the Porphyrin-coated Silicon Nanowire Field-effect Transistors

In this paper, we have analyzed electric potential distributions in undoped silicon nanowire field-effect transistor (Si-NW FET) with a back-gate configuration covered by organic compound - porphyrin. Specifically, we studied the 1D electrostatic potential along the different axes of the Si-NW FET for the subsequent investigation of electron transport characteristics. Reference 5, figures 6.

Keywords: silicone nanowire; field-effect transistor; porphyrin; electric potential.

Introduction

In recent years, Si-NW have been widely studied and used as building blocks for nanoscaled integrated circuits or sensors. Si-NW are good candidate for FET-based electrical sensors, because binding of charged entities can be monitored by the change of current through the channel of FET due to high surface-to-volume ratio [2], [6].

This paper addresses the problem of studying the electrophysical properties of porphyrin-coated NW-FETs. The aim of the paper is to analyze the electrostatic potential in back-gate undoped silicon nanowire Schottky barrier FETs for the subsequent electron transport characteristics.

Geometry of Porphyrin-Coated Silicon Nanowire FET

The device structure of Si-NW FET is similar to typical three-electrode transistor (Fig.1a), where Si-NW placed between a source and a drain electrode on an insulating SiO2 substrate [2]. Our model of Si-NW FET has nickel-silicide contacts as Schottky interfaces, which have been obtained due to diffusion of Ni into Si [1].

Fig. 1. Schematic images of porphyrin-coated Si-NW FET in 3D (a), Y-X (b) and Y-Z (c) cross section views
Fig. 1 b-c shows the schematic image of porphyrin-coated Si-NW FET in Y-X and Y-Z cross-sectional views, respectively. This device consists of Si-NW – working as conducting channel and NiSi2 - based NWs, working as source and drain contacts. The parameters for source V_S, drain V_D, gate voltages V_G, length of Si-NW channel L_{Si-NW}, length of NW L, the thickness of porphyrin layer t_{por}, the thickness of SiO_2 layer t_{SiO2}, NW diameter t_{NW}, and the thickness of oxide layer t_{ox} are shown in Fig. 1c.

Theoretical Framework

We can obtain the electric potential by solving the Poisson (1) equation with given boundary conditions and with given surface charge densities as:

\[ \nabla^2 V(r) = \frac{-\rho(r)}{\varepsilon_0 \varepsilon_r} \]  

(1)

where \( \nabla \) is the divergence operator, \( V(r) \) – 3D electric potential along the axis of the Si-NW, \( \rho(r) \) – space charge density, \( \varepsilon_0 \) and \( \varepsilon_r \) are vacuum permittivity and dielectric constant or relative electric permittivity, respectively.

The 1D electrostatic potential \( V(r) \) along the axis of the Si-NW has been obtained from the 3D electric potential after solving Poisson equation using finite element method (FEM) [5]. The geometry of the device was built and calculations of electrostatic potential were performed by dint of software COMSOL Multiphysics [4]. The boundary potentials for the source, drain and gate contacts are constant and equal \( V_S=0V \), \( V_D=0,1V \) and \( V_G=2V \).

Results and Discussion

Electrostatic potential distribution of the porphyrin-coated Si-NW FET from Fig. 1a has been calculated. Fig. 2 depicts the potential landscape with a gate potential \( V_G=2V \) and drain-source voltage \( V_{DS}=0,1V \).

![Fig. 2. Electrostatic potential distribution of porphyrin-coated Si-NW FET](image)

After modeling the device geometry we have obtained the distribution of the electric potential lengthwise the axis Z – along the Si-NW channel with the length of 1.0 \( \mu \)m (Fig. 3a) and along the porphyrin layer (Fig. 3b).

![Fig. 3. Distribution of the electric potential lengthwise the axis Z - along the Si-NW channel (a) and along the porphyrin layer (b)](image)

Fig. 4 depicts electric potentials distribution lengthwise the channel with the length of 1.0 \( \mu \)m for different gate voltages (\( V_G=-6V \ldots 14V \)).
Fig. 4. Electrostatic potential along the axis of the Si-NW channel for different values of gate voltages

Also we have considered electric potential distributions for other directions. Distribution of the electric potential lengthwise the axis X is shown in Fig.5.

We can observe electric potential across the metal NiSi₂ contacts (Fig.5a), across the NiSi₂/Si-NW interface (Fig.5b) and the Si-NW channel (Fig.5c). Electric potential across the Si-NW channel has nonuniform distribution in the middle of nanowire and on its edges. Drop of potential between Si-NW and Air is practically unessential in comparison with NiSi₂/Air and NiSi₂ - Si-NW/Air.

Fig.6 depicts electric potential distributions lengthwise the axis Y - across the structure with metal NiSi₂ (Fig.6a), across the structure with NiSi₂/Si-NW interface (Fig.6b) and Si-NW channel (Fig.6c). Potential fall across the structures with metal is more significant unlike the fall of potential across the structures with Si-NW. In addition, we observe electric potential rising from porphyrin edge for structures with metal NiSi₂ and NiSi₂/Si-NW, and unessential potential fall from porphyrin edge for structures with Si-NW.
Conclusions

The first step to create appropriate model of the Si-NW FETs sensor is to calculate the electrostatic potential along the axis of the Si-NW channel of the device. In this work, we have shown 3D distribution of electric potential in the porphyrin-coated Si-NW FETs. Also we have depicted 1D electric potential along the axis of the Si-NW channel for different values of gate voltages in the porphyrin-coated Si-NW FETs, that can enables ones to calculate the current through the channel of the device, using Landauer-Buttiker approach combined with the method of non-equilibrium Green’s functions [3], [5]. Such model permits to see how the change of geometrical parameters, external and internal factors will affect the current through NW of porphyrin-coated Si-NW FETs. The future work will involve obtaining the transfer characteristic and comparison the experimental data [1] with modeling results and adjust our model.

References

Аналіз одно- і трьохвимірного розподілу електричного потенціалу в польовому транзисторі на основі кремнієвого нанопроводу покритого порфірином

У даній роботі ми проаналізували розподіл електричного потенціалу в нелегованому польовому транзисторі на основі кремнієвого нанопроводу (ПТ з Si-НП) з конфігурацією нижнього за- твору, покритого органічним з'єднанням - порфірином. Зокрема, ми вивчили однорідний розподіл електростатичного потенціалу вздовж різних осей ПТ з Si -НП для наступних досліджень характеристик переносу електронів. Бібл. 5, рис. 6

Ключові слова: кремнієвий нанопровід; польовий транзистор; порфірин; електричний потенціал.

Список іспользованих источников
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