Твердотельная электроника

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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].

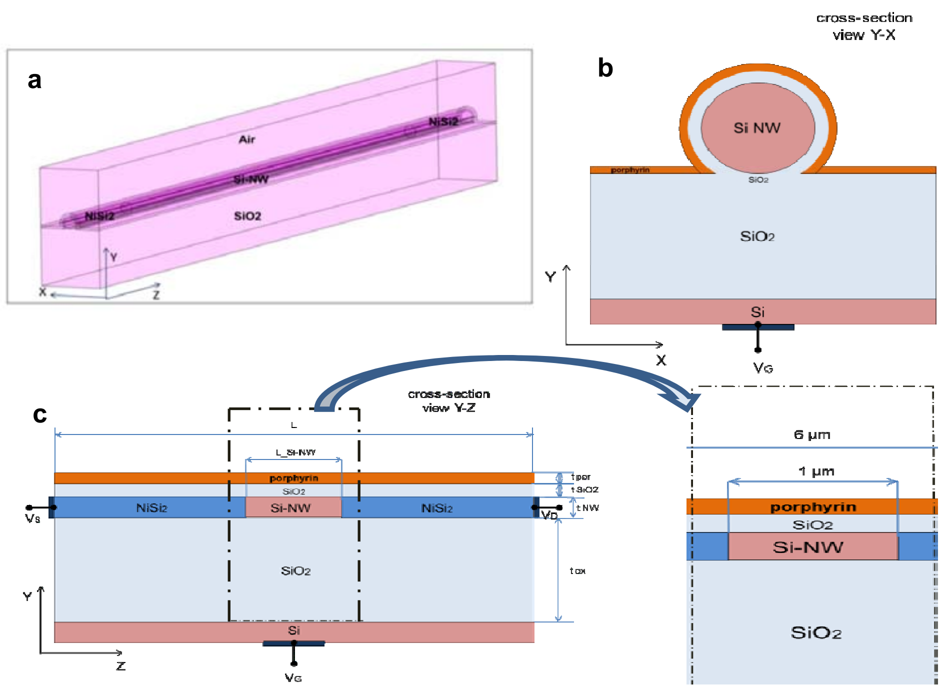

Fig. 1. Schematic images of porphyrin-coated Si-NW FET in 3D (a), Y-X (b) and Y-Z (c) cross section views

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 $NiSi_2$ - 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 $L_{Si\text{-}NW}$, 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:

$$\nabla^2 V(r) = -\frac{\rho(r)}{\varepsilon_0 \varepsilon_r} \qquad (1)$$

where ∇ is the divergence operator, $V(r)$ – 3D electric potential along the axis of the Si-NW, $\rho(r)$ – space charge density, ε_0 and ε_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 VG=2V and drain-source voltage VDS=0,1V.

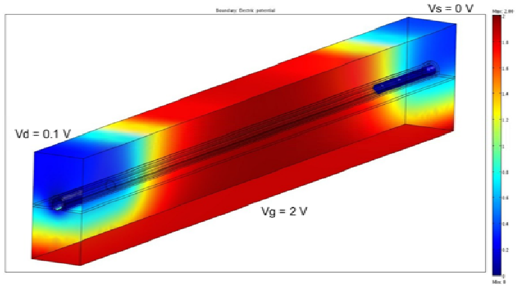

Fig. 2. Electrostatic potential distribution of porphyrin-coated Si-NW FET

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 μm (Fig.3a) and along the porphyrin layer (Fig.3b).

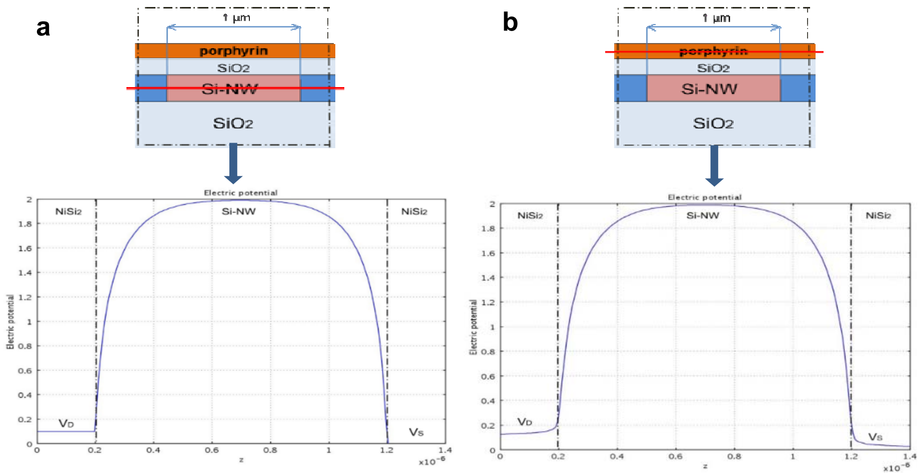

Fig. 3. Distribution of the electric potential lengthwise the axis Z - along the Si-NW channel (a) and along the porphyrin layer (b)

Fig. 4 depicts electric potentials distribution lengthwise the channel with the length of 1,0 μm for different gate voltages (Vg=-6V…14V).

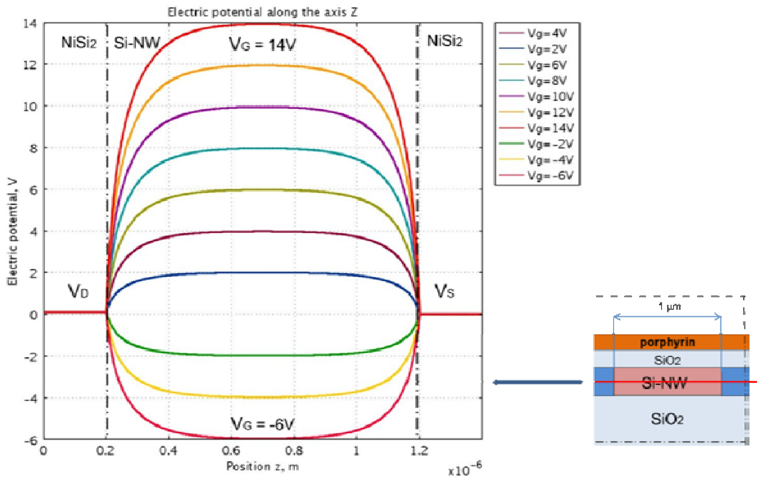

Fig. 4. Electrostatic potential along the axis of the Si-NW channel for different values of gate voltages

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

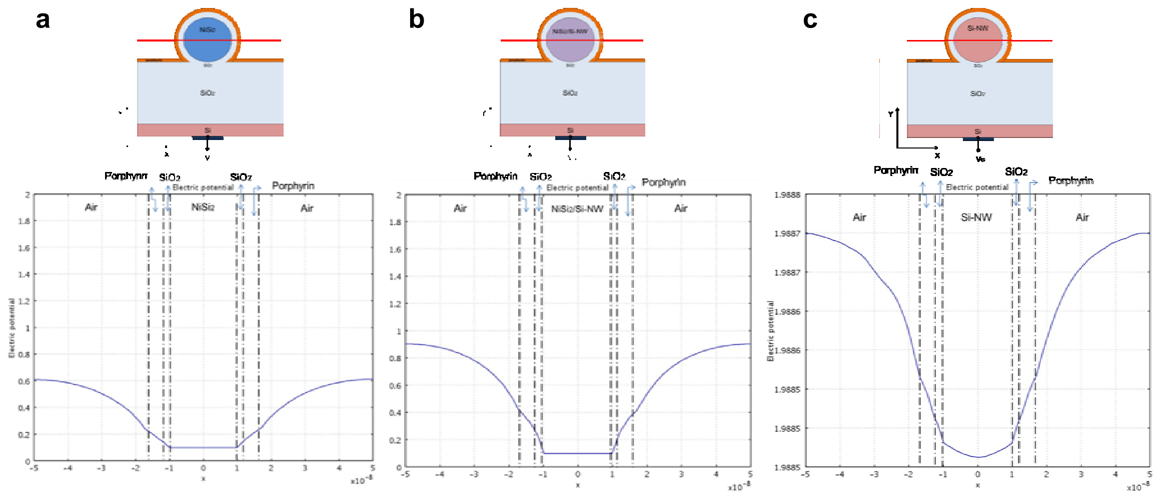

Fig. 5. Distribution of the electric potential lengthwise the axis X - across the metal $NiSi_2$ contacts (a), the $NiSi_2$/Si-NW interface (b) and across the Si-NW channel (c)

We can observe electric potential across the metal $NiSi_2$ contacts (Fig.5a), across the $NiSi_2$/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 $NiSi_2$/Air and $NiSi_2$ - Si-NW/Air.

Fig.6 depicts electric potential distributions lengthwise the axis Y - across the structure with metal $NiSi_2$ (Fig.6a), across the structure with $NiSi_2$/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 $NiSi_2$ and $NiSi_2$/Si-NW, and unessential potential fall from porphyrin edge for structures with Si-NW.

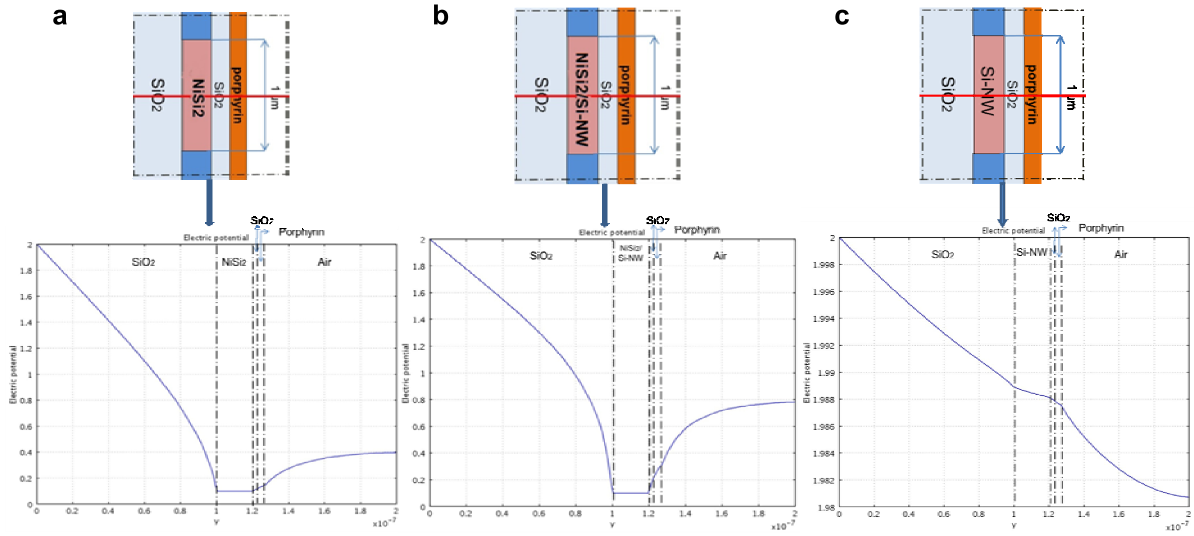

Fig. 6. Distribution of the electric potential lengthwise the axis Y - across the structure with metal $NiSi_2$ (a), the structure with $NiSi_2$/Si-NW interface (b) and Si-NW channel (c)

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.

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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 затвору, покритого органічним з'єднанням - порфірином. Зокрема, ми вивчали одномірний розподіл електростатичного потенціалу вздовж різних осей ПТ з Si -НП для наступних дослыджень характеристик переносу електронів. Бібл. 5, рис. 6

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

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Анализ одно- и трехмерного распределения электрического потенциала в полевом транзисторе на основе кремниевого нанопровода покрытого порфирином

В данной работе мы проанализировали распределение электрического потенциала в нелегированном полевом транзисторе на основе кремниевого нанопровода (ПТ с Si-НП) с конфигурацией нижнего затвора, покрытого органическим соединением - порфирином. В частности, мы изучали одномерное распределение электростатического потенциала вдоль различных осей ПТ с Si-НП для последующих изучений характеристик переноса электронов. Библ. 5, рис. 6.

Ключевые слова: *кремниевый нанопровод; полевой транзистор; порфирин; электрический потенциал.*

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