Sensing and Bio-Sensing Research 11 (2016) 45–51

Contents lists available at ScienceDirect

Sensing and Bio-Sensing Research

journal homepage: www.elsevier.com/locate/sbsr

Monolayer MoS_2 and WSe_2 Double Gate Field Effect Transistor as Super Nernst pH sensor and Nanobiosensor

Abir Shadman *, Ehsanur Rahman, Quazi D.M. Khosru

Department of Electrical and Electronic Engineering, Bangladesh University of Engineering and Technology, Dhaka 1000, Bangladesh

ARTICLE INFO

Article history:
Received 27 June 2016
Received in revised form 24 August 2016
Accepted 26 August 2016

Keywords:
Double gate FET
2D material
pH sensor
Nernst limit
Drift diffusion
Nanobiosensor

ABSTRACT

Two-dimensional layered material is touted as a replacement of current Si technology because of its ultra-thin body and high mobility. Prominent transition metal dichalcogenides (TMD), Molybdenum disulphide (MoS_2), as a channel material for Field Effect Transistor has been used for sensing nano-biomolecules. Tungsten diselenide (WSe_2), widely used as channel for logic applications, has also shown better performance than other 2D materials in many cases. pH sensor is integrated with Nanobiosensor most often since charges (value and type) of many biomolecules depend on pH of the solution. Ion Sensitive Field Effect Transistor with Silicon and III–V materials has been traditionally used for pH sensing. Experimental result for MoS_2 field effect transistor as pH sensor has been reported in recent literature. However, no simulation-based study has been done for single layer TMD FET as pH sensor or bio sensor. In this paper, novel MoS_2 and WSe_2 monolayer double gate FETs are proposed for pH sensor operation in Super Nernst regime and protein detection. In case of pH sensing bottom gate operation ensures these monolayer FETs operating beyond Nernst limit of 59 mV/pH. Besides pH sensing, the proposed monolayer FETs also show reasonably high sensitivity in sub threshold region as protein detector. Simulation results found in this work reveal that, scaling of bottom gate oxide results in better sensitivity for both pH and biosensor while top oxide scaling exhibits an opposite trend in pH sensing.

1. Introduction

Ion-sensitive field-effect transistor (ISFET) is one of the most common approaches to label free nanobiosensor. Piet Bergveld first introduced ISFET in 1970. It is similar to the metal oxide semi-conductor field effect transistor (MOSFET). The ISFET, also known as pH sensor, has been used to measure ion's concentrations (H^+ or OH^-) in a solution. The two dimensional layered ISFET works in same principle as silicon based ISFETs. Protonation/deprotonation of the OH groups on the gate insulator (Fig. 1(a)) depending on the pH value of the electrolyte, changes the dielectric surface charge. It is the basic principal of pH detection. Lower pH value promotes the protonation of the solution, generating positive surface charges on the dielectric while higher pH value does the opposite. The resultant surface charge and the electrolyte voltage applied through a reference electrode also known as fluid/front gate voltage determine the surface potential. At a particular gate and drain bias in a FET, the change in pH would result in a change in surface charge in the oxide-electrolyte interface thereby changing the conductance of the channel material. This change in conductance will be reflected in the change in sensor current that would ultimately change the threshold voltage of the FET. This completes the basic operating principle of pH sensor. The pH sensitivity (mV/pH) for a conventional ISFET is defined by the changes of threshold voltage (V_T) at a given amount of pH changes. However, the pH sensitivity is always less than the well-known Nernst limit of 59 mV/pH for single gate operation. As reported in the literature [1,2], the limit in single-gated ISFET sensors can be breached by using the double gated field effect transistors. Most of the works until now of super-Nernst sensor involve silicon on insulator technology. In this work, we are proposing and studying monolayer TMD DGFET super-Nernst pH sensor for the first time. Because of highly scaled thickness up to an atomic plane and dangling bond free pristine surface [3,4], 2-D semiconducting transition metal dichalcogenides, such as MoS_2 and WSe_2, have been considered as prospective channel material for low power CMOS devices [5]. Monolayer MoS_2 and WSe_2 having considerable band gap (1.8 and 1.6 eV respectively [6]) results in higher I_{ON}/I_{OFF} ratio than the zero band gap graphene [7]. This property makes these materials suitable for low-power logic applications. Deblina Sarkar et al. [7] have recently demonstrated MoS_2 FET pH sensor. The work revealed that the lack of a band gap in graphene fundamentally limits sensitivity of graphene based sensor also. In this work the thickness of top and bottom gate oxides for both the TMD FETs have been varied from which it is found that increasing the thickness of top oxides results in reduced sensitivity while the trend is opposite for bottom oxide. This trend is also captured in the literature [1] for the Si FET. It is found that, with the simplifications presented in Section 2, inherent upper limit of pH sensitivity for these two TMD FET sensors is quite close to each other. This work has also investigated

* Corresponding author.
E-mail address: abir08@eee.buet.ac.bd (A. Shadman).

http://dx.doi.org/10.1016/j.sbsr.2016.08.005

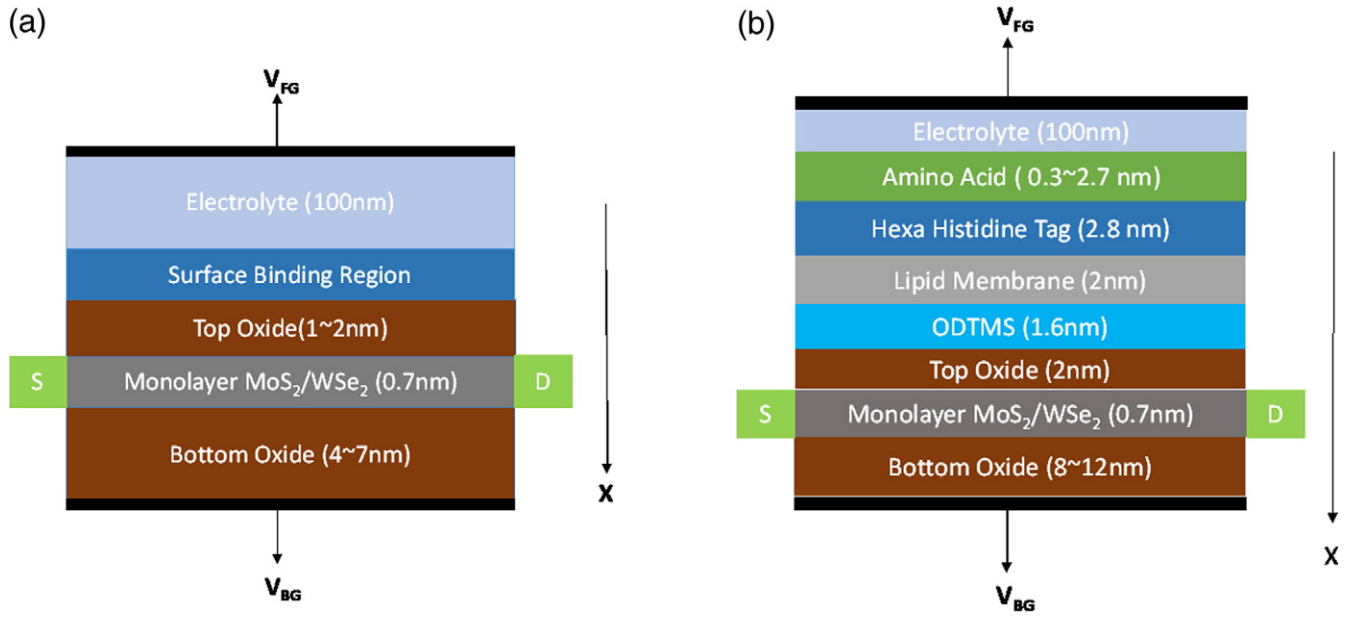

Fig. 1. (a) Simple Schematic representation of the pH sensor used in this work. (b) Simple Schematic structure of the biomolecule (amino acid) sensor used in this work. Here SiO_2 is used as top and bottom oxide for both pH and biosensor. None of the devices shown in this figure is drawn to scale.

a novel application of these materials in sensing biomolecules like protein. A comparative study of their sensitivity dependence on physical parameter like oxide thickness and device operation regime is carried out to maximize their detection capability in biosensor application. In this work we have developed a self-consistent Schrodinger Poisson solver which incorporates Boltzmann distribution in the electrolyte region to determine spatial charge and electrostatic potential distributions within the device for both pH and biomolecule sensor. In an attempt to provide more realistic prediction of the device physics simplification like Debye-Hückel approximation was avoided. The quantum mechanical charge density in the semiconductor was also taken into account.

2. Device structure & simulation methodology

Fig. 1(a) shows the schematic of the conventional double gate FET pH sensor used in this paper. Its channel material is single layer transitional metal dichalcogenide (monolayer MoS_2 and WSe_2). Transitional metal dichalcogenides are new type of materials that are being analyzed extensively as a prospective material to replace Si technology. Thickness of monolayer WSe_2 and MoS_2 has been considered 0.7 nm [8] and 0.65 nm [9] respectively in the literature. Although it is also common to treat the whole class of TMDC material with a thickness of 0.65 nm [10]. Gate dielectric is kept SiO_2 on both sides of the channel for this work. However, the simulation procedure [1] used in this work can easily take into account of various dielectrics. Here, fluid/front gate voltage, V_{FG} is kept 1 V for all simulations. In addition, Back gate voltage, V_{BG} is varied from 1 V to 5 V for operation over the Nernst limit. Top gate oxide is varied from 1 to 2 nm while the bottom gate oxide is varied from 4 to 7 nm. Single layer transition metal dichalcogenides' parameters have been taken from various references [11–15].

The electrolyte-top gate oxide interface is functionalized with surface groups (^{-}OH). Protons (H^+) in electrolyte react with these surface groups (-OH) which causes protonation and deprotonation. As a result of these reactions the net charge of -OH groups respond to the change of pH of the solution. The protonation/deprotonation of -OH groups are taken in to account by the surface binding model. According to the model, the chemical reactions occurring on the silicon oxide surface are as follows

$$\begin{aligned} SiOH + H_s^+ &\Longleftrightarrow SiOH_2^+ \\ SiO^- + H_s^+ &\Longleftrightarrow SiOH \end{aligned} \tag{1}$$

where H_s^+ represents the proton density near the surface region. The equilibrium constants for each of these reactions are described by the following equations:

$$\begin{aligned} \frac{[SiOH][H_s^+]}{[SiOH_2^+]} &= K_a \\ \frac{[SiO^-][H_s^+]}{[SiOH]} &= K_b \end{aligned} \tag{2}$$

The surface proton density H_s^+ is related to the bulk proton density H_B^+ at the solution by the Boltzmann distribution such that

$$\begin{aligned} [H_s^+] &= [H_B^+]\exp(-q\Phi_0/k_BT) \\ \Phi_0 &= \Phi_{x=0^+} - V_{FG} \end{aligned} \tag{3}$$

where Φ_0 is the electrostatic potential difference between the surface and the bulk electrolyte. The potential of the bulk electrolyte is fixed by the fluid gate (FG) bias. The bulk proton density $[H_B^+]$ is governed by pH of the electrolyte such that $pH = -\log_{10}[H_B^+]$. Now the net charge density of top oxide surface group can be expressed as

$$\sigma_{OH} = q\left([SiOH_2^+] - [SiO^-]\right) \tag{4}$$

In addition, the total density of the surface group is

$$N_s = [SiOH] + [SiOH_2^+] + [SiO^-] \tag{5}$$