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Quantum ballistic analysis of transition metal dichalcogenides based double gate junctionless field effect transistor and its application in nano-biosensor

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To reduce the thermal budget and the short channel effects in state of the art CMOS technology, Junctionless field effect transistor (JLFET) has been proposed in the literature. Numerous experimental, modeling, and simulation based works have been done on this new FET with bulk materials for various geometries until now. On the other hand, the two-dimensional layered material is considered as an alternative to current Si technology because of its ultra-thin body and high mobility. Very recently few simulation based works have been done on monolayer molybdenum disulfide based JLFET mainly to show the advantage of JLFET over conventional FET. However, no comprehensive simulation-based work has been done for double gate JLFET keeping in mind the prominent transition metal dichalcogenides (TMDC) to the authors' best knowledge. In this work, we have studied quantum ballistic drain current-gate voltage characteristics of such FETs within non-equilibrium Green's function (NEGF) framework. Our simulation results reveal that all these TMDC materials are viable options for implementing state of the art Junctionless MOSFET with emphasis on their performance at short gate lengths. Besides evaluating the prospect of TMDC materials in the digital logic application, the performance of Junctionless Double Gate trilayer TMDC heterostructure FET for the label-free electrical detection of biomolecules in dry environment has been investigated for the first time to the authors' best knowledge. The impact of charge neutral biomolecules on the electrical characteristics of the biosensor has been analyzed under dry environment situation. Our study shows that these materials could provide high sensitivity in the sub-threshold region as a channel material in nano-biosensor, a trend demonstrated by silicon on insulator FET sensor in the literature. Thus, going by the trend of replacing silicon with these novel materials in device level, TMDC heterostructure could be a viable alternative to silicon for potentiometric biosensing.

1. Introduction

With the MOSFET dimensions shrinking, we no longer can consider long channel behavior due to undesirable side effects [1]. The depletion widths of source and drain junctions are becoming comparable to the channel length because of the

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shortening of channel length. This readily causes the punch-through effect [2]. Increasing channel doping can come to the rescue. However, it will increase the threshold voltage. Scaling down of gate oxide thickness can be a solution to the problem. Again, tunneling and other quantum mechanical effects narrow down the chances of ideal scaling rule. Hence, with best scaling control, optimization of the scaled down devices is not possible with the unwarranted so-called short channel effects (SCE). Many techniques such as Gaussian doping profile, gate stack, source/drain design, FinFET architectures with multi-gates, and alternative channel material beside silicon have been proposed to overcome various SCEs and enhance device performance [2–4]. However, there are manufacturing problems related to some of the alternative techniques. Junctionless Field Effect Transistors (JLFETs) is thought to overcome fabrication challenges related to abrupt p-n junctions in state-of-the-art CMOS technology which might open a new era in the technology of nanoscale MOSFETs [5–7]. With the seminal work done by J. P. Colinge et al. [8], much more research on this new concept was done [5,9,10]. JLFET is reported to show excellent subthreshold slope (SS), small drain induced barrier lowering (DIBL), low leakage current, high I_{ON}/I_{OFF} ratio, etc. [5,8–12]. For inversion mode device, inversion channel at the interface between channel and gate oxide is formed above the threshold voltage, and flat band voltage is below the threshold voltage. In contrast, for JLFET which is an accumulation-mode device, flat-band voltage is above the threshold voltage, and the device is fully depleted below threshold voltage. Numerous analytical models and simulations have been done for JLFETs with various geometries for bulk materials.

On the other hand, because of highly scaled thickness up to an atomic plane and pristine surface without dangling bond [13,14], 2-D semiconducting transition metal dichalcogenides (TMDC), such as MoS_2 and WSe_2, have been considered as prospective channel materials for low power CMOS devices [15]. Monolayer TMDCs such as MoS_2 and WSe_2 have an appreciable band gap (1.8 and 1.6 eV respectively [6]) resulting 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. In this work, we have done a quantum ballistic evaluation of some widely used monolayer TMDC (MoS_2, $MoSe_2$, WS_2, and WSe_2) based JLFETs. Although some assessments of MoS_2 JLFET can be found in recent literature [16,17], it was done mainly to show the superiority of JLFET over conventional FET while the analysis with the other TMDC materials is still missing. Hence a detailed comparative study of different TMDC JLFETs would provide better understanding and optimization of their performance.

Besides its application in logic circuit, the excellent performance of TMDC JLFET has led to the further investigation of this structure in 'More than Moore Technology' in this work. Integrating the task of biochemical sensing with microelectronics and integrated circuits has been an extensive field of research in recent past. Specifically, the early detection of biomarkers indicative of lethal diseases like cancers has necessitated the need for the design of robust, selective and highly sensitive biosensors. Electronic detection of biomolecule at a very low concentration with little or no sample preparation has been an extensive field of research in recent literature. Potentiometric biosensors have been found to detect analytes like vascular endothelial growth factor (VEGF) molecules even in femtomolar limits in a dry environment [18]. Moreover, potentiometric biosensing in the dry environment has shown better sensitivity over a wet environment where the sensitivity is limited by Debye screening caused by electrolyte ions [19]. Given the prospects of a potentiometric biosensor in detecting bio-analytes, there has been a highly prospective field of ongoing research regarding the performance improvement of this type of sensor.

Layered van der Waals materials, such as transition metal dichalcogenides, few layers thick or exfoliated down to a single layer, have become the subject of extensive research in recent times [20,21]. Stacking multiple layers on top of each other of these materials also leads to interesting changes in electronic properties [22,23]. Besides bilayer 2D heterostructures, trilayer TMDC heterostructures based on MoS_2 have also been studied using first principle simulations [24]. Though monolayer and trilayer TMDC materials have been investigated [25,26] for potentiometric biosensing in a microfluidic environment to detect charged biomolecules, such biosensors cannot detect charge neutral biomolecules and suffer from sensitivity reduction caused by Debye screening. Dielectric Modulated FET (DMFET) approach employed in this work for biomolecules detection is different from other familiar methods found in recent literature regarding detection technique and device structures. For example, A. Gao [27] et al. presented a novel biosensor based on a silicon nanowire tunneling field-effect transistor (SiNW-TFET). It was experimentally demonstrated for point of care diagnostics. It functionalizes the surface of SiNW to capture biomolecule, not like conventional DMFET. In another experimental work [28], F. Puppo et al. showed the capability of SiNW-FET to detect antigen in brain tumor extract with high sensitivity specifically. Graphene-based FET used as an aptasensor has been reported as effective in lead detection in children blood [29]. Gold nanoparticle-decorated graphene FET biosensor [30] is reported to have the capability of achieving label-free, ultrasensitive and highly selective detection of miRNA with high sensitivity as well as a high selectivity. Sub-femtomolar cancer biomarker detection is also achieved with these G-FETs [31]. However, these transistor-based sensors work on the watery environment. In an aqueous environment, the charge of the bioparticle to be detected is partially screened by the different ions presents in the electrolyte solution [19] which is well known as Debye screening. Moreover, the charge of such biomolecules in an aqueous environment is highly dependent upon the pH of the solution which requires a very well controlled pH based solution so that biomolecules contain detectable charges. Hence a new detection technique based on the dielectric permittivity of biomolecules has been found in recent literature which is free from the problems of aqueous solution based bio-detection. Specifically, R. Narang et al. [32,33] has proposed Dielectric Modulated Tunnel FET as a biosensor and studied analytical modeling and sensitivity analysis for label-free detection. Tunnel FET sensor is expected to result in better sensitivity compared to FET-based sensor [33]. Various metrics like $I_{on}, SS, \Delta V_{th}$ etc. have been investigated [33] to measure sensitivity. Being inspired by their works, we have further investigated the prospect of such biomolecule detection technique in a different device structure with an entirely different channel made of 2D materials. In this work, we focused on $\frac{\Delta I}{I}$, a metric which has been found to provide the best sensitivity among all.