Electrically Doped WTe_2 Tunnel Transistors

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***Abstract*—In this work, the performance of an electrically doped monolayer WTe_2 tunnel field-effect (TFET) transistor is investigated by means of full band quantum transport simulations. The atomistic simulations predict an ON-current above 100 uA/um and a SS below 10 mV/dec for a channel length of 13nm and V_{DD} of 0.5V. The impact of the design parameters such as oxide thickness and dielectric constant is discussed in detail.**

I. Introduction

In the last decade, tunnel field effect transistors (TFETs) have attracted a lot of attention for their promise as low power transistors [1], [2], [3]. One of the main challenges ahead of TFETs are their low ON-currents compared to ultra-scaled MOSFETs [4]. Recently, it has been shown that transition metal dichalcogenide (TMD) material based TFETs have the potential for providing high ON-currents, if compared to other TFETs, while keeping the subthreshold swing (SS) less than the conventional Boltzmann limit of 60 mV/dec at room temperature [5]. Among TMD materials, WTe_2 was found to be the best candidate for high performance TFET application owing to its lower bandgap and effective mass [5]. Despite the fact that a high chemical doping of the source contact is crucial for having a high performance TFET [5], chemical doping method in itself comes with a suit of drawbacks. Chemical doping of 2D materials has been proven challenging although some initial work has been done to identify the right chemical species and doping methods. Moreover, the chemical doping can introduce defects and dopant states in the bandgap which can degrade the OFF-state performance of the device [6], [7]. To avoid these problems, an *electrically doped* WTe_2 TFET is proposed here as a candidate for high performance TFET applications. The impact of the device design on the performance of this TFET is discussed in this article.

II. Simulation methodology

The atomistic quantum transport simulations use a sp^3d^5 2nd nearest neighbor tight-binding (TB) model with spin-orbit coupling to describe the WTe_2 Hamiltonian and a self-consistent Poisson-NEGF (Non-equilibirum Green's Function) method to calculate the current-voltage characteristics of the device. The material properties of simulated monolayer WTe_2 are listed in Table I. The structure of a monolayer WTe_2 TFET is shown in Fig. 1. Each gate has a length of 13nm, and there is no spacing between the gates. An electrically doped pn junction can be created in this structure by applying biases of opposite polarity on the two gates [6]. A source-to-drain voltage V_{DS} of 0.5V is applied. The total thickness of the device (shown as T_{tot} in Fig.1) including the body thickness of the monolayer WTe_2 equals 4.4nm. All of the

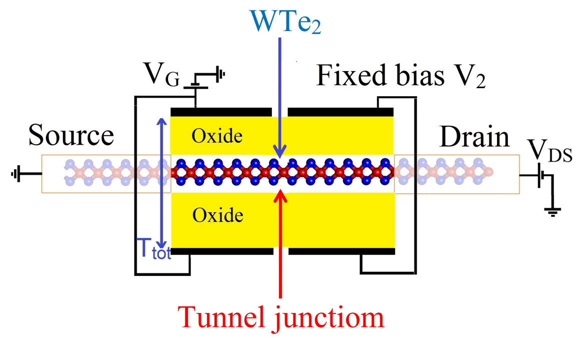

Fig. 1. Physical structure of an electrically doped double gated TFET based on monolayer WTe_2.

transport simulations have been performed with the nanodevice simulation tool NEMO5 [8], [9], [10].

III. Results

Fig. 2 shows transfer characteristics of the WTe_2 TFET for different device thicknesses ($T_{tot} = 2t_{ox} + t_{body}$ as shown in Fig. 1). The ON-current strongly depends on the oxide thickness. Increasing the oxide thickness by a factor of 2, reduces the ON-current values by approximately 2 orders of magnitude. Notice that an ON-current of 130 uA/um can be achieved with a T_{tot} of 2.9nm which is a high ON-current for a TFET. This value of ON-current was previously obtained in *chemically doped* WTe_2 TFETs with a doping level of 1e20 cm^{-3}. Accordingly, one can extract the *oxide thickness* of electrical gating equivalent to a specific *chemical doping* level in the chemically doped devices.

Fig. 3 depicts the effect of variation in the oxide dielectric constant (ϵ_{ox}) on the transfer characteristics of WTe_2 TFETs. It is apparent that the dielectric constant of the oxide does not have any significant impact on the performance of electrically doped TFETs. From Fig. 2 and 3, one can conclude that the oxide thickness is much more important in the case of the electrically doped TFETs. This means that the concept of *equivalent oxide thickness* (EOT) is not applicable to electrically doped TFETs which is in contrast to the conventional knowledge that EOT is the major player in transistors.

TABLE I. WTe_2 MATERIAL PROPERTIES: BAND GAP (E_g), ELECTRON AND HOLE EFFECTIVE MASSES (m_e^* AND m_h^*), AND IN-PLANE AND OUT-OF-PLANE RELATIVE DIELECTRIC CONSTANTS (ϵ_r^{in} AND ϵ_r^{out}) [5], [14].

Parameters	E_g [eV]	m_e^* [m_0]	m_h^* [m_0]	ϵ_r^{in}	ϵ_r^{out}
WSe_2	0.75	0.37	0.3	5.7	3.3

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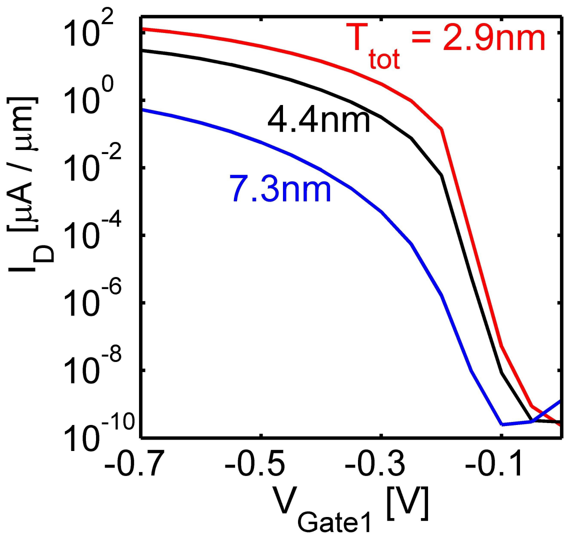

Fig. 2. Transfer characteristics of WTe_2 TFETs with different oxide thicknesses and the same oxide dielectric constant (ϵ_{ox}=20). V_{DS} and V_2 are fixed to 0.5V and 0.65V, respectively.

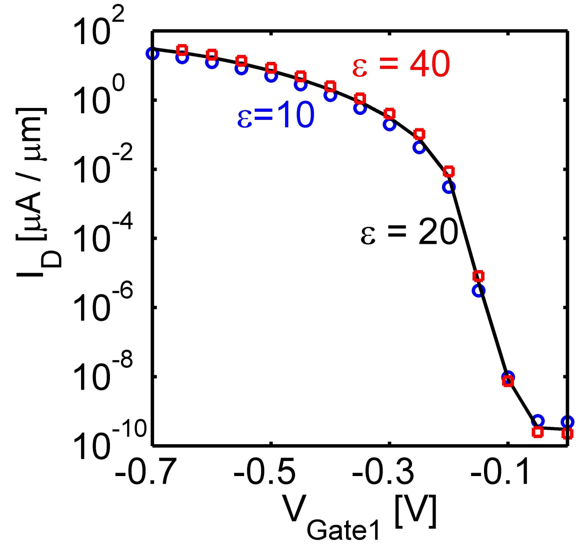

Fig. 3. Transfer characteristics of WTe_2 TFETs with different oxide dielectric constants and the same oxide thickness (T_{tot}=4.4). V_{DS} and V_2 are fixed to 0.5V and 0.65V, respectively.

Recently, a new scaling theory has been introduced for this novel class of electrically doped devices [6]. According to this scaling theory, the main factors determining the performance of electrically doped devices are the physical thickness of the oxide and spacing between the gates. The natural scaling length λ in electrically doped devices can be written as [6]:

$$\lambda = \frac{2t_{ox} + t_{body} + S/4}{\pi} = f(t_{ox}) \tag{1}$$

where S is the distance between the gates and t_{ox} and t_{body} are the oxide and body thicknesses, respectively. Notice that the scaling length λ does not depend on ϵ_{ox}, but only on t_{ox}. The electric field at the tunnel junction (E_T) is inversely proportional to λ.

$$E_T \propto \frac{1}{2t_{ox} + t_{body} + S/4} \tag{2}$$

As a result, increasing the oxide thickness decreases the electric field and the ON-current. The WTe_2 TFET simulation results are in good agreement with this scaling theory. Fig. 4 shows the conduction band profile of two WTe_2 TFETs. The solid lines show the band profile with T_{tot} of 2.9nm (red line) and 4.4nm (blue line). The circles are the analytic profile obtained from the previously introduced scaling theory [6]:

$$V(x) = \frac{V_1 - V_2}{2} exp\left(-\frac{\pi}{T_{tot}}(x - x_M)\right) + V_2 \tag{3}$$

where V_1, V_2 are the potential of the left and right gates respectively and x_M is the position of the interface between the gates. The band profile obtained from (3) matches well with the atomistic simulations. Notice that this independence of performance from the oxide dielectric constant is not usually observed in chemically doped devices in which EOT and source doping levels are the major players [11], [12], [13].

IV. Conclusion

In conclusion, in this work a high performance electrically doped TFET based on monolayer WTe_2 is proposed. It is shown that the physical thickness of the oxide is crucial in the case of electrical doping and using a high-K material cannot improve the situation significantly. This observation implies that in the case of electrically doped devices, an oxide with the largest bandgap would be favorable, and not necessarily with the highest dielectric constant. The large bandgap of the oxide would suppress the gate leakage for small oxide thicknesses required for high performance TFETs.

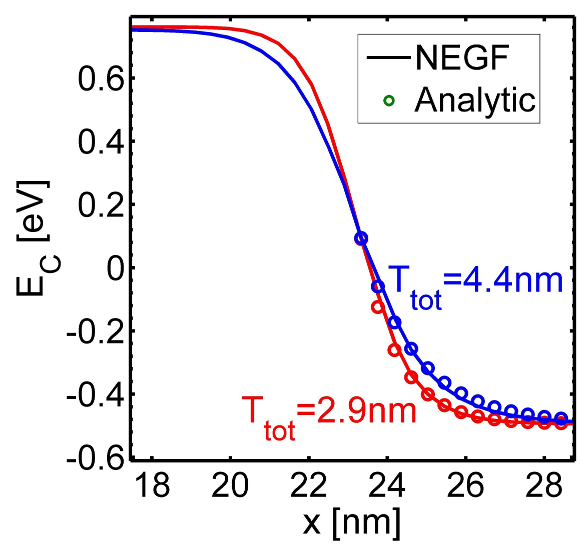

Fig. 4. The conduction band profiles of WTe_2 TFETs with different oxide thicknesses and the same oxide dielectric constant (ϵ_{ox}=20). V_{DS} and V_2 are fixed to 0.5V and 0.65V, respectively.

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