Negative differential resistance in monolayer WTe$_2$ tunneling transistors

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Abstract
We report theoretical investigations of quantum transport in monolayer transition metal dichalcogenide (TMDC) tunneling field effect transistors (TFETs). Due to the specific electronic structure of TMDC WTe$_2$, a transmission valley is found in the conduction band (CB). For a proper choice of the doping, gate and supply voltages the WTe$_2$ TFET can produce a giant negative differential resistance (NDR) with a peak to valley ratio as large as 10$^3$. The mechanism of NDR is identified to be due to a transport-mode bottleneck, i.e., the band to band tunneling from the valence band of the source is partially blocked by a transmission valley of the CB of the drain. More generally, our calculations show that electronic structures of at least six TMDC materials possess the transmission valley.

Keywords: transition metal dichalcogenide, tunneling field effect transistors, negative differential resistance

(Some figures may appear in colour only in the online journal)

1. Introduction

Recently a new class of two-dimensional (2D) material—the monolayer (ML) transition metal dichalcogenides (TMDCs)—has received great attention due to their significant potential as the channel material in emerging nanoelectronic devices [1, 2]. 2D TMDCs such as ML MoS$_2$ and WTe$_2$, are semiconductors having a direct band gap larger than 1 eV, they possess reasonable carrier mobility and are stable in ambient conditions [3, 4]. These properties make 2D TMDCs interesting for achieving high on-off ratio for field effect transistor (FET) applications. Existing works also suggest many other applications including in biosensors, displays, and logical circuits [5–9]. Beside MOSFET, a very interesting direction is to investigate TMDCs as the channel material for tunneling field effect transistors (TFETs) [10–12] which is important for low power electronics.

In this work, by atomistic theoretical analysis we discover that TFETs made of 2D TMDC material WTe$_2$ can behave as a negative differential resistance device (NDR). NDR is a nonlinear transport phenomenon where an increasing bias voltage $V$ results to a decreasing current $I$ so that the differential resistance $dI/dV < 0$. NDR gives rise to electronic oscillations widely applied for multi-functional electronic operation in circuits [13–15]. NDR is typically observed in semiconductor devices [16–19] in the resonant tunneling regime where the bias voltage pushes the resonant quantum level to below the bottom of the conduction band (CB) thereby diminishing the current. NDR was also observed in STM measurements involving a tip and a substrate separated by a vacuum barrier [20]. There, the NDR was understood as due to the on-and-off alignment of narrow features in the density of states (DOS) of the two parts—tip and substrate, across the tunnel barrier. More recently, possible NDR was reported in FETs of ML MoS$_2$ where the NDR was due to the narrow energy band-width of the first CB [21].

The mechanism of NDR in WTe$_2$ TFETs reported here is a combined result of the misalignment of DOS with band to band tunneling. We found that for WTe$_2$ TFETs there is a transmission bottleneck going from the valence band (VB) of the source to the CB of the drain, and this bottleneck gives
The current of WTe$_2$ TFETs is a tunneling current which is very sensitive to the transmission valley. Therefore, the TFET can reach very high peak-valley current ratio (PVCR) as large as 10$^3$. This is significantly larger than that of semiconductor devices such as SiGe diodes [13] where PVCR is around 300. Importantly, our calculations show that electronic structures of at least six TMDC materials possess a similar transmission valley.

2. Device structure and simulation details

The simulated WTe$_2$ double-gate device structure is illustrated in figure 1. A 2 nm thick HfO$_2$ oxide with dielectric constant $\varepsilon = 25$ is used as the gate insulator. The channel material is WTe$_2$. The reason we chose WTe$_2$ is that the material has a smaller band gap and also a smaller carrier effective mass compared with other TMDCs such as MoS$_2$, MoSe$_2$, MoTe$_2$, WS$_2$ and WSe$_2$ [22]. As a result, a relatively larger tunneling current can be reached for WTe$_2$ TFETs. Nevertheless, since the electronic structures of these TMDC materials are all similar to that of WTe$_2$, the NDR physics to be presented below is quite general. Following [10], the dielectric constant of WTe$_2$ is taken to be $\varepsilon_{WTe_2} = 7$. The source and drain are well doped to p-type and n-type, respectively, and the channel under the gate is intrinsic. Experimental realizations of n-type or p-type TMDC FETs have recently been achieved [23–26], hence the p–i–n TFET structure should be experimentally feasible. The length of source/drain and channel are 8 and 10 nm, respectively.

Figure 1. (a) Schematic structure of a double-gate WTe$_2$ TFET using HfO$_2$ as the gate oxide. The TFET consists of three parts: a p-type source, an intrinsic channel and an n-type drain. (b) Atomic structure along the armchair direction of WTe$_2$. The dopant densities in the p-doped source and n-doped drain are the same, 1.8 x 10$^{13}$ cm$^{-2}$. (c) Schematic band diagram along the transport direction showing the band to band tunneling.

Along armchair direction. The band to band tunneling physics is illustrated in figure 1(c).

The Hamiltonian of WTe$_2$ is described by a three band tight binding model [22] which in the low energy range reproduces the band structure in the entire Brillouin zone obtained by density functional theory (DFT) with generalized gradient approximation (GGA). We have also carried out DFT calculations using the HSE hybrid functional [27, 28]. The HSE band gap is found to be 1.48 eV which is 0.41 eV larger than the GGA gap. On the other hand, the band dispersions of HSE and GGA agree with each other. The ballistic device characteristics are calculated by self-consistently solving the Poisson equation and the open boundary Schrödinger equation within the nonequilibrium Green’s function formalism. After the self-consistent computation is finished, the drain current can be obtained from the Laudauer equation:

$$I_D = \frac{2e}{hL} \int dE \sum_k T(E, k) \left[ \delta(E - E_D) - \delta(E - E_S) \right],$$

where $L$ is the channel width, $T(E, k)$ is the transmission coefficient and integrated over the wave vector $k$ perpendicular to the transport direction, and $\delta(E)$ is the source (drain) Fermi distribution function. In our calculations we focus on the ballistic transport properties of WTe$_2$ TFETs at room temperature. Because the simulated channel length is shorter than the phonon limited mean free path [29], it is reasonable to neglect the electron-phonon scattering. In our simulation of the double-gate TFETs, a 2 nm thick HfO$_2$ oxide layer is applied so that the device has a good gate control. Practically, the gate oxide layer may be thicker, the contact resistance and parasitic capacitance are inevitable. Hence gate control is deteriorated and a larger gate or bias voltage is experimentally necessary.
3. Results and discussion

Figure 2(a) presents the calculated zero bias transmission spectrum $T(k, E)$ by color coding in the $k$--$E$ plane, where $k$ is the wave-vector and $E$ is the energy of the electron. $T(k, E)$ gives the number of available transport channels per cross section of the unit-cell and we obtain conductance by $G(E) = G_0 \sum T(k, E)/L$ where $G_0 = 2e^2/h$ is the conductance quanta and $L$ is the width of the unit-cell. Note that at about 0.50--0.8 eV above the bottom of CB, there is a region in the $(k, E)$ plane having no transport channel as indicated by the dark blue region in the dashed box. This leads to a transmission or conductance valley—a minimum of $G(E)$, in figure 2(b) at $E \sim 1.24$ eV. This feature of the channel material gives rise to NDR. Qualitatively, in the p--i--n TFET, carriers tunnel from the VB of the p-type source through the intrinsic channel to the CB of the n-type drain (see figure 1(c)). If carriers happen to tunnel to the transmission valley as indicated by the large arrows in figure 2(a), a small current is expected. By sweeping the drain voltage such a scenario can be established resulting to NDR. Importantly, our calculations show that the transmission valley which is responsible for the NDR exists in at least six different TMDC materials in the form of MX$_2$ (Where M = Mo, W; X = S, Se, Te) and the transmission valley information of these materials is listed in table 1. The NDR effect in these ML TMDC TFETs is therefore quite general and not limited to the specific band structure of WTe$_2$.

Having understood the equilibrium $T(k, E)$ and the qualitative possibility of NDR, now analyze the $I$--$V$ characteristics of the drain current $I_D$ versus drain bias $V_D$. In our simulation, the Fermi level is set at the middle of the band gap for the intrinsic channel. The work function of the gate electrode is neglected which results in a shift of the threshold voltage. Figure 3 shows the calculated $I_D$ versus $V_D$ for the WTe$_2$ TFET at different gate voltages $V_G$. We observe that the WTe$_2$ TFETs have very good on-off properties. At the drain voltage $V_D = 0.4$ V, the on-off ratio reaches $4.6 \times 10^4$ with a gate voltage window equal to the drain voltage. Because of the tunneling physics, the drain current is small, at about $1.2 \times 10^{-3} \mu A \mu m^{-1}$.

Dependong on the gate voltage $V_G$, several $I_D - V_D$ curves in figure 3 show NDR where $I_D$ decreases with the increase of $V_D$. At a small gate voltage $V_G = 0.2$ V, there is no NDR and $I_D$ simply increases with $V_D$ showing the typical TFET performance [30]. Increasing $V_G$ to 0.4 V, $I_D$ first increases with $V_D$ and then saturates, afterward it decreases with $V_D$. The NDR persists until $V_G$ reaches roughly 1.2 V. Note that the band gap of WTe$_2$ is 1.07 eV, thus the thermonic current above the CB of the source can be neglected and $I_D$ is essentially a tunneling current.

We shall analyze NDR by calculating the local density states (LDOS) and the current density. We start by considering the case of $V_G = 0.2$ V which has no NDR, figure 4 shows its LDOS and current density at two values of drain bias $V_D$. For $V_D = 0.1$ V, $I_D$ is overwhelmingly contributed by direct tunneling from the VB of the source to the CB of the drain, figure 4(a). This direct tunneling is mainly in the energy window between the chemical potentials of the source and drain, and contributes a very small current as shown in figure 4(b). By increasing $V_D$ to 0.6 V, the CB edge in the drain is pushed downward hence the tunneling barriers from source VB to drain CB, and from channel VB to drain CB, become thinner. From the LDOS in figure 4(c), we find that the tunneling barrier from the source VB through channel VB to the drain CB is the thinnest, which leads to much larger current density as shown in figure 4(d). Compared with the case of $V_D = 0.1$ V (figure 4(b)), the current density at $V_D = 0.6$ V is three orders of magnitude larger. The current is mainly composed of tunneling current from channel VB to drain CB around $E_{FD} = -E_F$. Therefore at $V_G = 0.2$ V, $I_D$ increases with $V_D$ due to the thinning of tunneling barrier and there is no NDR.

When the gate voltage is increased to $V_G = 0.6$ V, the bands in the channel are pushed downward as shown in figure 5(a). We observe that the CB edge of the channel is now blow the Fermi energy of the drain. Hence at $V_D = 0.1$ V, $I_D$ is mainly composed of tunneling current from source VB to channel CB as shown in figures 5(a) and (b), which is different from that at $V_G = 0.2$ V. As $V_D$ is increased to 0.6 V, we observe that $I_D$ comes mainly from the energy region

| Table 1. $E_g$ is the band gap energy, $E_p$ is the energy difference between the conductance valley energy minimum at $k = 2\pi/3L$ and conduction band minimum, and $E_n$ is the conductance valley width at $k = 2\pi/3L$. From the valley width $E_n$ the operating window of drain voltage for NDR can be roughly estimated. |

| Material | $E_g$ (eV) | $E_p$ (eV) | $E_n$ (eV) |
|----------|----------|----------|----------|
| MoS$_2$  | 1.66     | 0.56     | 0.13     |
| WS$_2$   | 1.81     | 0.77     | 0.05     |
| MoSe$_2$ | 1.43     | 0.49     | 0.05     |
| WSe$_2$  | 1.54     | 0.61     | 0.11     |
| MoTe$_2$ | 1.07     | 0.35     | 0.20     |
| WTe$_2$  | 1.07     | 0.53     | 0.26     |

Figure 3. $I_D - V_D$ characteristics of monolayer WTe$_2$ TFETs at different gate voltages ($V_G$).
−0.3 eV < E < −0.1 eV rather than the energy region around the Fermi energy (E = 0) as shown in figure 5(d). From the LDOS in figure 5(c), we find that E = 0 in the drain corresponds to the conductance valley in CB where it has less available transmission channels as shown in figure 2(b). In this energy range, carriers tunnel from VB of the source to CB of the drain as demonstrated in figure 2(a), but there are fewer available channels in the drain at this energy range. Therefore even though the tunneling barrier is thinner, the tunneling current becomes smaller as shown in figure 5(d). As a result, I_D decreases when V_D increases from 0.1 to 0.6 V, resulting to NDR. Further increasing V_D, I_D keeps decreasing until the role played by the CB valley of the drain diminishes. For V_G = 0.6 V, the calculated I_D − V_D curve up to V_D = 1.0 V is plotted in figure 6, showing a very prominent NDR. We note that I_D begins to increase when V_D reaches 0.8 V. The peak to valley ratio of the NDR reaches 10^3 which is a very significant value.

4. Conclusion

In summary, we have investigated electronic transport in 2D WTe_2 TFETs and found a very strong NDR effect. The NDR is due to the existence of a ballistic conductance valley in the CB of the material. Tunneling from VB of the source to CB of the drain can be blocked by the valley leading to small drain current hence NDR. The NDR can be varied by the drain bias, and the peak to valley ratio of the drain current can be as large as 10^3. These properties should allow the design of low bias NDR device using the 2D WTe_2 TFETs. Finally, as presented above we found that at least five other TMDC materials have a similar transmission valley as that of WTe_2. Therefore the reported NDR is quite general for this class of materials.
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