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Selection Mechanism of Band Alignment in 2D $p^+/n$ Tunnel FET

Tunnel field effect transistors (TFETs) are promising for the low power switching FETs which can overcome the theoretical limitation of the subthreshold swing ($\text{S.S.} = 60 \text{ meV/dec}$) for conventional MOSFETs [11]. 2D-materials are expected to be suitable for TFETs because 2D-TFETs have short tunnel distance defined by van der Waals heterointerface, thereby gaining higher on-current than that for conventional 3D-TFETs. Although the $p^+/n$ heterostructure is necessary to achieve the low S.S., doping technique is still under development for both interstitially and chemically. Recently, we have found that $p^+$/WSe₂ doped chemically by WO₃ can be stabilized in air by transferring it on h-BN, and observed band-to-band tunneling (BTBT) current in the $p^+$/WSe₂/4-layer (L) MoS₂ heterostructure [2]. However, its band alignment could not be changed from type II to type III even by applying the sufficient gate bias, although type-III band alignment is necessary to gain large BTBT current. In this study, $p^+$/WSe₂/MoS₂ heterostructures consisting of 1 - 5L MoS₂ were fabricated and their transport properties were investigated in order to reveal the MoS₂ thickness dependence on the band alignment of charge-transfer-type $p^+/n$ heterostructure and achieve type-III band alignment.

$p^+$/WSe₂ needs to be stable in air for the source of TFET. After forming WSe₂/WO₃ by O₃ annealing at 200 °C for 1 h, WO₃ side is transferred onto h-BN and $p^+$/WSe₂ is stabilized. After that, MoS₂ with suitable thickness (1 - 5L) is chosen by its contrast on PDMS and the $p^+$/WSe₂/MoS₂ heterostructures were fabricated via dry transfer method using PDMS under the alignment system. Ni/Au was deposited as source/drain electrodes after the electrode pattern formation by an electron beam lithography. Then, Y₂O₃ buffer layer (1.5 nm), Al₂O₃ oxide layer (~30 nm) and Al top-gate electrode were formed. Figure 1 shows (a) schematic illustration and (b) optical image of the top-gate $p^+$/WSe₂/2L-MoS₂ TFET device.

Firstly, the $p^+$/WSe₂/3L-MoS₂ device with 30-nm-Al₂O₃ was fabricated. This device consists of thinner MoS₂ and Al₂O₃ than those in the previous $p^+$/WSe₂/4L-MoS₂ device with 60-nm-Al₂O₃ showing the type-II band alignment [2]. Figure 2 shows the diode properties of 3L-MoS₂ device with various top gate voltage ($V_{TG}$) at 20 K. The current at reverse bias is due to BTBT because minority carriers have been suppressed at sufficiently low temperature. When $V_{TG}$ is -9 ~ 15 V, BTBT current can flow at reverse bias and negative differential resistance (NDR) trend is clearly observed as the intersection of BTBT current and diffusion current at forward bias. The appearance of NDR trend indicates that type-III band alignment is achieved.

Figure 3(a) compares $I_{DS}$-$V_{TG}$ at $V_{SD} = -2$ V (reverse bias) between the 3L-MoS₂ and previous 4L-MoS₂ devices. Higher on-current can be obtained in the 3L-MoS₂ device than that in the 4L-MoS₂ device mainly owing to type-III band alignment. S.S. of the 3L-MoS₂ device does not depend on the temperature and is increased by increasing $I_{DS}$, as shown Fig. 3(b). These characteristics also support that the current at reverse bias is indeed due to BTBT and $p^+$/WSe₂/3L-MoS₂ device is operated as TFET.

In order to reveal the relationship between MoS₂ thickness and the band alignment in $p^+$/WSe₂/MoS₂ device, Figure 4(a) compares diode properties of $p^+$/WSe₂/1-5L MoS₂ devices at $V_{TG} = 15$ V and 20 K. The 3L-MoS₂ device is only the type-III, while the other devices are the type-II because 1, 2 and 4L MoS₂ devices show BTBT current only at large reverse bias and the 5L-MoS₂ device does not show BTBT current even for reverse bias of -2 V. The brown arrows in Fig. 4(a) are defined as BTBT onset voltage ($V_{BTBT}$), which implies band offset between the conduction band minimum (CBM) for MoS₂ and the valence band maximum (VBM) for $p^+$/WSe₂. So $V_{BTBT}$ can be modulated by $V_{TG}$ and ideally reaches 0 V when band alignment is changed from type II to type...
III for the 3L-MoS₂ device, as shown in Fig. 4(b). However, $V_{\text{BTBT}}$ saturates before reaching 0 V for the other devices, although it is evident that Fermi level ($E_F$) in MoS₂ is sufficiently modulated for all the thickness cases. This suggests that the restriction to type II results from $p^+$-WSe₂, not from MoS₂, that is, $E_F$ in WSe₂ is apart from VBM due to the $p$-doping reduction. For this $p$-doping reduction in WSe₂, two different origins can be considered. One is electron transfer from MoS₂; the other is that the top gate modulates $p^+$-WSe₂ as well as MoS₂.

Figure 5 illustrates band alignments controlled by above-mentioned two different physical origins. When $p^+$-WSe₂ is contacted with MoS₂, electron is transferred from MoS₂ to WSe₂ and $E_F$ of WSe₂ uniformly increases because WSe₂ is doped by electron transfer to WOₓ. Because the amount of transferred electron increases with increasing MoS₂ thickness, $E_F$ of WSe₂ also changes by MoS₂ thickness and band alignment become type II for 4 and 5L-MoS₂ devices, which is shown by dotted blue line in Fig. 5. The band alignment change due to this charge transfer can be seen as (I) in Fig. 4(b). In this consideration, type III should be obtained for 1L and 2L. However, when MoS₂ thickness is become thin like 1L and 2L, WSe₂ is also expected to be modulated by the top gate. Therefore, by applying $V_{\text{TG}}$, $E_F$ in WSe₂ as well as MoS₂ is modulated at the same time, resulting to the type II from type III by decreasing MoS₂ thickness, as shown by a dotted orange line in Fig. 5 and (II) in Fig. 4(b). Because of these two different origins for $p$-doping reduction in WSe₂, only 3L MoS₂ shows type III.

Through this study, it is revealed that band alignment of $p^+$-WSe₂/MoS₂ TFET is controlled by the two different physical origins, that is, $F$ modulation in WSe₂ by $V_{\text{TG}}$ and electron transfer from MoS₂. Since both origins depends on the MoS₂ channel thickness, the band alignment is quite sensitive to the MoS₂ thickness. This kind of drastic change with MoS₂ thickness because $p^+$-doping from WOₓ is not high enough.

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Figures

Figure 1: (a) Schematic illustration and (b) optical image of the $p^+$-WSe₂/3L-MoS₂ TFET device.

Figure 2: Diode properties of $p^+$-WSe₂/3L-MoS₂ TFET at

Figure 3: (a) $I_{\text{DS}}$-$V_{\text{TG}}$ curves of 3L- and 4L-MoS₂ devices. (b) S.S. as functions of $I_{\text{DS}}$

Figure 4: (a) Diode properties and (b) BTBT onset voltage as functions of $V_{\text{TG}}$ for $p^+$-WSe₂/1 - 5L MoS₂ devices.

Figure 5: $V_{\text{BTBT}}$ as a function of MoS₂ thickness with the illustration of band alignment at $V_{\text{TG}} = 15$ V.