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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 (*S.S.* = 60 meV/dec) for conventional MOSFETs [1]. 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^+-WSe$_2$ doped chemically by WO$_x$ can be stabilized in air by transferring it on *h*-BN, and observed band-to-band tunneling (BTBT) current in the p^+-WSe$_2$/4-layer (L) MoS$_2$ 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^+-WSe$_2$/MoS$_2$ heterostructures consisting of 1 - 5L MoS$_2$ were fabricated and their transport properties were investigated in order to reveal the MoS$_2$ thickness dependence on the band alignment of charge-transfer-type p^+/n heterostructure and achieve type-III band alignment.

p^+-WSe$_2$ needs to be stable in air for the source of TFET. After forming WSe$_2$/WO$_x$ by O$_3$ annealing at 200 °C for 1 h, WO$_x$ side is transferred onto *h*-BN and p^+-WSe$_2$ is stabilized. After that, MoS$_2$ with suitable thickness (1 - 5L) is chosen by its contrast on PDMS and the p^+-WSe$_2$/MoS$_2$ 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, Y$_2$O$_3$ buffer layer (~1.5 nm), ALD-Al$_2$O$_3$ 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^+-WSe$_2$/2L-MoS$_2$ TFET device.

Firstly, the p^+-WSe$_2$/3L-MoS$_2$ device with 30-nm-Al$_2$O$_3$ was fabricated. This device consists of thinner MoS$_2$ and Al$_2$O$_3$ than those in the previous p^+-WSe$_2$/4L-MoS$_2$ device with 60-nm-Al$_2$O$_3$ showing the type-II band alignment [2]. **Figure 2** shows the diode properties of 3L-MoS$_2$ 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-MoS$_2$ and previous 4L-MoS$_2$ devices. Higher on-current can be obtained in the 3L-MoS$_2$ device than that in the 4L-MoS$_2$ device mainly owing to type-III band alignment. *S.S.* of the 3L-MoS$_2$ 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^+-WSe$_2$/3L-MoS$_2$ device is operated as TFET.

In order to reveal the relationship between MoS$_2$ thickness and the band alignment in p^+-WSe$_2$/MoS$_2$ device, **Figure 4(a)** compares diode properties of p^+-WSe$_2$/1-5L MoS$_2$ devices at V_{TG} = 15 V and 20 K. The 3L-MoS$_2$ device is only the type-III, while the other devices are the type-II because 1, 2 and 4L MoS$_2$ devices show BTBT current only at large reverse bias and the 5L-MoS$_2$ 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 MoS$_2$ and the valance band maximum (VBM) for p^+-WSe$_2$. 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-MoS_2 device, as shown in **Fig. 4(b)**. However, V_{BTBT} saturates before reaching 0 V for the other devices, although it is evident that Fermi level (E_F) in MoS_2 is sufficiently modulated for all the thickness cases. This suggests that the restriction to type II results from p^+-WSe_2, not from MoS_2, that is, E_F in WSe_2 is apart from VBM due to the *p*-doping reduction. For this *p*-doping reduction in WSe_2, two different origins can be considered. One is electron transfer from MoS_2; the other is that the top gate modulates p^+-WSe_2 as well as MoS_2.

Figure 5 illustrates band alignments controlled by above-mentioned two different physical origins. When p^+-WSe_2 is contacted with MoS_2, electron is transferred from MoS_2 to WSe_2 and E_F of WSe_2 uniformly increases because WSe_2 is doped by electron transfer to WO_x. Because the amount of transferred electron increases with increasing MoS_2 thickness, E_F of WSe_2 also changes by MoS_2 thickness and band alignment become type II for 4 and 5L-MoS_2 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 MoS_2 thickness is become thin like 1L and 2L, WSe_2 is also expected to be modulated by the top gate. Therefore, by applying V_{TG}, E_F in WSe_2 as well as MoS_2 is modulated at the same time, resulting to the type II from type III by decreasing MoS_2 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 WSe_2, only 3L MoS_2 shows type III.

Through this study, it is revealed that band alignment of p^+-WSe_2/MoS_2 TFET is controlled by the two different physical origins, that is, E_F modulation in WSe_2 by V_{TG} and electron transfer from MoS_2. Since both origins depends on the MoS_2 channel thickness, the band alignment is quite sensitive to the MoS_2 thickness. This kind of drastic change with MoS_2 thickness happens because p^+-doping from WO_x is not high enough.

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References: [1] A. M. Ionescu *et al*., Nature 2011, **479**, 329. [2] J. He *et al*., Adv. Electron. Mater. 2018, **4**, 1800207.

Figures

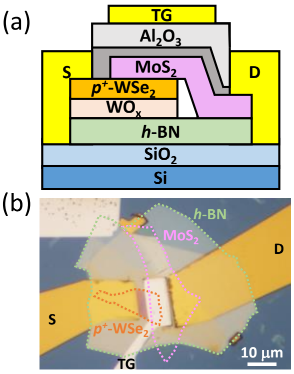

Figure 1: (a) Schematic illustaration and (b) optical image of the p^+-WSe_2/2L-MoS_2 TFET device.

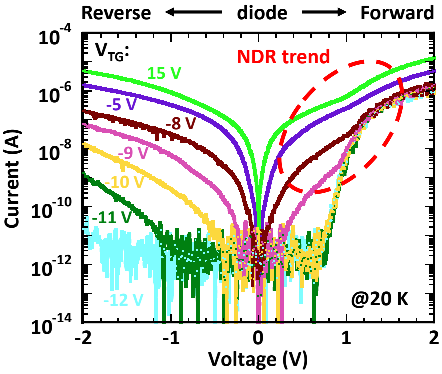

Figure 2: Diode properties of p^+-WSe_2/3L-MoS_2 TFET at

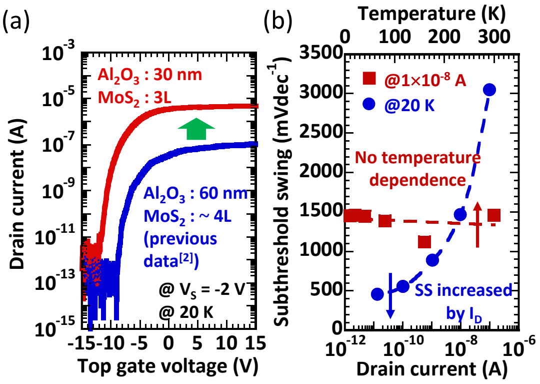

Figure 3: (a) I_{DS}-V_{TG} curves of 3L- and 4L-MoS_2 devices. (b) *S.S.* as functions of I_{DS}

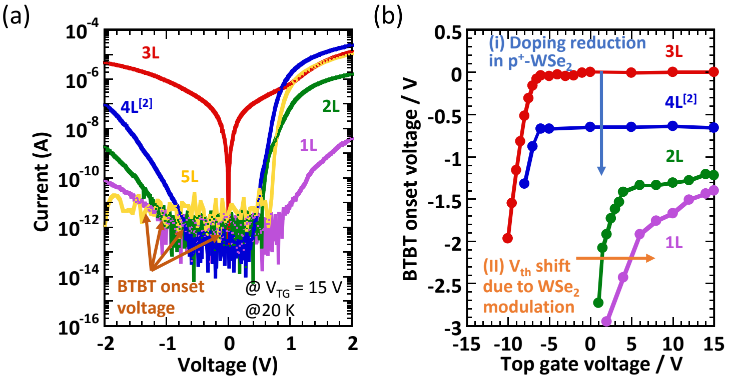

Figure 4: (a) Diode properties and (b) BTBT onset voltage as functions of V_{TG} for p^+-WSe_2/1 - 5L MoS_2 devices.

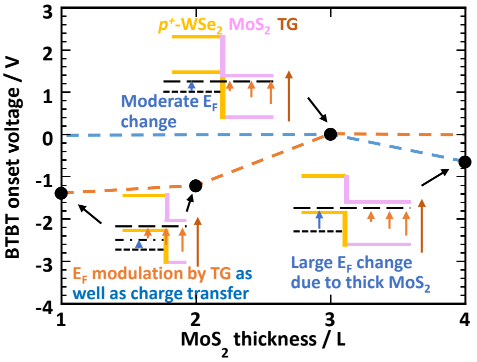

Figure 5: V_{BTBT} as a function of MoS_2 thickness with the illustration of band alignment at V_{TG} = 15 V.