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Trapped charge modulation at the MoS_2/SiO_2 interface by a lateral electric field in MoS_2 field-effect transistors

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Abstract

Controlling trapped charges at the interface between a two-dimensional (2D) material and SiO₂ is crucial for the stable electrical characteristics in field-effect transistors (FETs). Typically, gate-source bias has been used to modulate the charge trapping process with a narrow dielectric layer with a high gate electric field. Here, we observed that charge trapping can also be affected by the lateral drain-source voltage ($V_{\rm DS}$) in the FET structure, as well as by the gate-source bias. Through multiple $V_{\rm DS}$ sweeps with increasing measurement ranges of the $V_{\rm DS}$, we demonstrated that the charge trapping process could be modulated by the range of the applied lateral electric field. Moreover, we inserted a hexagonal boron nitride (h-BN) layer between the MoS₂ and SiO₂ layer to explore the charge trapping behavior when a better interface is formed. This study provides a deeper understanding of controlling the electrical characteristics with interface-trapped carriers and lateral electrical fields in 2D material-based transistors.

1. Introduction

Atomically thin two-dimensional (2D) materials such as MoS₂, MoSe₂, WS₂, and WSe₂ have attracted tremendous attention as innovative nanoelectronic materials [1–4]. Among the 2D materials, MoS₂ is an excellent channel material for realizing 2D-based field-effect transistors (FETs) due to its outstanding electrical characteristics [5, 6] and intrinsic band gap feature (~1.9 eV for monolayer and 1.2 eV for bulk MoS₂) [7, 8]. In addition to these advantages, the MoS₂ FET shows good electrical stabilities from thermal [9, 10] and mechanical [11, 12] alterations, which are essential requirements for FETs. In spite of the innate stabilities of MoS₂, unstable electrical characteristics could be observed, caused by extrinsic sources. For example, trapped charges existing at the interface between MoS₂ and a gate dielectric layer (such as SiO₂) have been considered one of the dominant sources incurring electrically unsteady states [13, 14]. Occasionally, deliberate charge trapping at the interface between MoS₂ or charge injection into SiO₂ has been used for materializing 2D material-based memory devices [15, 16]. Typically, to control trapping or detrapping electrons, gate-source bias has been used with a thin gate dielectric layer where a high gate electric field can be built [15, 16]. In our study, we observed that the charge trapping process in MoS₂ FETs could also be controlled by the measurement range of the lateral drain-source voltage (V_{DS}). Understanding altering electrical characteristics by the V_{DS} sweep range is considerably important for the realization of the stable electrical performance of FETs.

In addition to their advantages, trapped charges can function as Coulomb scattering sites and provide an effective gate-source bias, which can lead to fluctuating conductance [13, 14]. Therefore, large hysteresis in MoS₂ FETs induced by trapped charges can be an obstacle to practical applications in electronic devices. To avoid such obstacles, inserting a hexagonal boron nitride (h-BN) layer between MoS₂ and SiO₂ has been proposed to





improve the interface condition due to its atomically flat surface without dangling bonds [17, 18]. Then, high carrier mobility was successfully achieved in 2D material-based FETs with such an h-BN buffer layer [17, 18].

Here, charge trapping and detrapping processes at the interface between MoS₂ and SiO₂ layers in MoS₂ FETs were investigated through multiple V_{DS} sweeps with increasing measurement ranges of the V_{DS} . We observed that electrons became trapped at the MoS₂/SiO₂ interface in the V_{DS} measurement range of up to 105 V, and then trapped electrons started to be withdrawn by a lateral electric field of ~67.3 kV cm⁻¹. Moreover, we fabricated a MoS₂ FET by inserting an h-BN buffer layer between the MoS₂ and SiO₂ layers and compared the electrical characteristics of these MoS₂ FETs with those of MoS₂ FETs without an h-BN layer. The carrier mobility of the MoS₂ FET with the h-BN layer showed a higher value (~52.7 cm² V⁻¹ · s⁻¹) than those of all the MoS₂ FETs without the h-BN layer characterized in this work (ranging from 0.5 cm² V⁻¹ · s⁻¹ to 46.0 cm² V⁻¹ · s⁻¹), and the hysteresis disappeared when a better interface was formed between the semiconductor and gate dielectric layer.

2. Results and discussion

Figure 1(a) shows a schematic of the multilayer MoS₂ FET device and the molecular structure of MoS₂. An optical image of a fabricated MoS₂ FET is shown in figure 1(b). The thickness of the mechanically exfoliated MoS₂ film (~3.8 nm) was measured by atomic force microscopy (AFM). The Raman peak positions of E^{1}_{2g} and A^{1}_{g} correspond to the in-plane and out-of-plane lattice vibrations, respectively, and the value of the frequency difference (~24 cm⁻¹) indicates an uncontaminated multilayer MoS₂ sheet (figure 1(c)) [19]. Detailed fabrication processes are explained in the supplementary information (figure S1 is available online at stacks.iop.org/NANOF/3/011002/mmedia) and experimental details section. Figures 1(d) and (e) exhibit the transfer curve (drain-source current versus gate-source voltage, $I_{DS}-V_{GS}$) and the output curve (drain-source roltage roltage, $I_{DS}-V_{DS}$) of a multilayer MoS₂ FET measured in vacuum (~10⁻⁴ Torr) at room temperature. These data showed good *n*-type semiconductor behavior with a high on/off ratio of over 10⁹ and carrier mobility of 29.3 cm² V⁻¹ · s⁻¹. The carrier mobility as a function of V_{GS} is indicated in figure S2 in the supplementary information. Note that all the mobility values in this work





signify the maximum values measured at $V_{\rm DS}$ in the linear region. The carrier mobility (μ) was calculated by the formula $\mu = (dI_{\rm DS}/dV_{\rm GS}) \times [L/(WC_iV_{\rm DS})]$, where $W(\sim 25 \ \mu\text{m})$ is the channel width, $L(\sim 15.6 \ \mu\text{m})$ is the channel length, and $C_i = \varepsilon_o \varepsilon_r / d = 1.3 \times 10^{-4} \text{ F} \cdot \text{m}^{-2}$ is the capacitance between the MoS₂ and heavily doped Si back gate per unit area. Here, ε_o is the vacuum permittivity, $\varepsilon_r (\sim 3.9)$ is the dielectric constant of the SiO₂ dielectric, and *d* is the thickness (270 nm) of the SiO₂ layer.

To investigate the trapped charge effect on electrical characteristics, we applied a finite gate-source voltage pulse (denoted as V_{GS,before}) of -40 V or 40 V for one second before the actual measurement and then examined the output curve at a zero gate-source voltage ($V_{GS} = 0$). Figure 2(a) indicates that two different electrical configurations were observed: one with a higher saturation current (represented by filled circular symbols) and another with a lower saturation current (represented by open circular symbols), which are controlled by $V_{\rm GS, before}$ (figure 2(a)). The origin of the two separate configurations can be explained by the effect of trapped electrons induced by V_{GS,before}. Because the MoS₂ channel and SiO₂ dielectric form an incomplete interface, trapped electrons could exist at the interface of MoS₂/SiO₂, which influences the channel current flow. This result is consistent with previous studies in which $V_{\rm GS}$ was used to control charge trapping by taking advantage of a narrow dielectric layer (a few hundred nanometers) with a high gate electric field [13, 14]. To classify two different configurations clearly, we applied the strong voltage of $V_{GS,before}$ (-40 V or 40 V). As shown in figure 2(b), when $V_{\text{GS,before}} = -40$ V was applied, the trapped electrons escaped from the trap sites at the interface to the MoS₂ channel. On the other hand, when $V_{GS,before} = 40$ V was applied, some free electrons were trapped at the trap sites at the interface. These two electrical configurations are denoted as the unoccupied-traps state and occupied-traps state, respectively (figures 2(a) and (b)). The trapped electrons induced by $V_{GS,before}$ caused Coulomb scattering with the free carriers (conduction electrons) in the MoS2 channel and acted as a negative gate-source bias during the measurement, even at a fixed value of $V_{GS} = 0$ V, leading to reduced conductivity in the MoS₂ channel (figure 2(a)).

Similar to the above method using a gate-source voltage, trapped charges can also be controlled by a lateral electric field (i.e. a drain-source voltage). Figure 3(a) shows the output curves of a multilayer MoS₂ (12 nm-thick) FET under a series of $V_{\rm DS}$ sweeps with an increasing measurement range from 40 V (from 0 V to 40 V) to 130 V (from 0 V to 130 V) at a fixed $V_{GS} = 0$ V. Each V_{DS} sweep with increasing measurement ranges was performed in sequence without interval time. We fixed $V_{\rm GS} = 0$ V, so that the channel current does not flow too much in the MoS₂ channel, even at high V_{DS} range, which avoids a permanent breakdown phenomenon by the Joule heating effect. When the measurement range increased from 40 V (from 0 V to 40 V, black filled circular symbols) to 105 V (from 0 V to 105 V, violet filled circular symbols), the saturation current gradually decreased from ~130 nA to ~30 nA, as shown in figures 3(a) and (b). In contrast, the saturation current continuously increased in $V_{\rm DS}$ sweeps from the measurement range of above 110 V (from 0 V to 110 V, gray open circular symbols). The decreased saturation current during the $V_{\rm DS}$ sweeps up to the measurement range of 105 V is ascribed to the charge trapping process because the free electrons can be trapped in the trap sites at the MoS₂/SiO₂ interface, and so the trapped electrons negatively affect the saturation current on the next $V_{
m DS}$ sweep measurement (represented by the trapping process shown in figure 3(b)). After the V_{DS} sweep of 105 V (violet filled circular symbols), the trapped electrons started to be detrapped out of the trap sites owing to the strong lateral drainsource electric fields, which resulted in an increased saturation current in the next $V_{\rm DS}$ sweep measurement ranges from 110 V to 130 V (represented by the detrapping process shown in figure 3(b)). To calculate the energy levels of trap sites, we utilized the simplified Poole–Frenkel model in which the trapped charge can begin to





Figure 3. (a) $I_{\rm DS} - V_{\rm DS}$ curves under multiple $V_{\rm DS}$ sweeps with increasing measurement $V_{\rm DS}$ ranges from 40 V (from 0 V to 40 V) to 130 V (from 0 V to 130 V) at $V_{\rm GS} = 0$ V. (b) Saturation current as a function of the measurement $V_{\rm DS}$ range at $V_{\rm GS} = 0$ V. Black, red, blue, green, magenta, orange, dark green, and violet filled circular symbols correspond to the $V_{\rm DS}$ sweep ranges of 40, 50, 60, 70, 80, 90, 100, and 105 V, respectively, for the trapping process. Gray, pink, cyan, light pink, and navy open circular symbols correspond to the $V_{\rm DS}$ sweep ranges of 110, 115, 120, 125, and 130 V, respectively, for the detrapping process.

escape the potential barrier via thermionic-field emission at $V_{\rm DS} = 105$ V. From the calculation, it was determined that the trapped electrons in trap sites would be located more than 72 meV away from the conduction band, which is in accordance with a previous study [20] (see figure S3 for details in the supplementary information). The schematics for describing the trapping and detrapping processes by multiple $V_{\rm DS}$ sweeps with different measurement $V_{\rm DS}$ ranges are illustrated in the supplementary information (figure S4). Note that the abrupt increase in the channel current above 110 V is due to the avalanche breakdown process under strong lateral electric fields [21].

To clearly identify whether the origin of the change in saturation current in response to the different $V_{\rm DS}$ sweep ranges was due to trapped charges, we further investigated and compared the saturation currents obtained from the repeated measurements under the occupied-traps state or unoccupied-traps state. Before the actual measurement, the occupied-traps or unoccupied-traps states were formed by applying $V_{GS,before} = 40$ V or -40 V, respectively (figures 4(a) and (b)). In the occupied-traps state (after applying $V_{GS,before} = 40$ V), the saturation current gradually increased and became saturated during the multiple V_{DS} sweeps from 0 V to 105 V at a fixed value of $V_{\rm GS} = 0$ V, as shown in figure 4(a). This phenomenon is attributed to the detrapping process by the high lateral drain-source electric field (~67.3 kV cm⁻¹). Note that quite a high $V_{\rm DS}$ over 105 V was required for the detrapping process due to the long channel length (\sim 15.6 μ m) of our FET, and the range of the V_{DS} depends on the channel length of each device. The electrons escaped from the trap sites by the multiple $V_{\rm DS}$ sweeps, which gradually changed from the occupied-traps state to the unoccupied-traps state. The schematics of the detrapping processes by the multiple V_{DS} sweeps, explaining the results of figure 4(a), are illustrated in the supplementary information (figure S5). On the other hand, in the unoccupied-traps state (after applying $V_{GS, before} = -40$ V), the saturation currents did not change during the multiple $V_{\rm DS}$ sweeps because of a lack of electrons in the trap sites at the interface, as shown in figure 4(b). Figure 4(c) summarizes the values of the saturation currents during multiple $V_{
m DS}$ sweeps in the occupied-traps and unoccupied-traps states. The difference in saturation current after the six repeated measurements between the occupied-traps state (~38 nA) and unoccupied-traps state (~67 nA) signifies the influence of the trapped electrons remaining after repeated measurements.

As mentioned in the introduction, understanding the control of trapped electrons is required for the stable electrical characteristics of MoS_2 -based transistors or memory devices. In particular, a better interface between MoS_2 and the dielectric layer should be formed to avoid fluctuating conductance by trapped charges. In this manner, we inserted the h-BN layer between MoS_2 and SiO_2 to form an ideal interface without dangling bonds. Figures 5(a) and (b) show the schematics of the multilayer MoS_2 FETs without and with h-BN between the MoS_2 and SiO_2 layers. The thicknesses of the multilayer MoS_2 for the data of figures 5(a) and (b) were found to be ~12 nm and ~18 nm, respectively. We could not use the same MoS_2 thickness to compare the charge trapping behavior in figure 5. Note that the electrical characteristics can be dependent on the MoS_2 thickness [22, 23], but the influence of charge trapping by the difference in the MoS_2 thickness has been reported to be unclear and disputable [24–27]. Therefore, a further study exploring charge trapping. The thickness of the h-BN layer for the data shown in figure 5(b) was ~19 nm. The optical images and Raman spectrum for the fabricated MoS_2 FET with the h-BN layer are shown in the supplementary information (figure S6). Figures 5(c) and (d) indicate





traps state and unoccupied-traps state).

the transfer curves of the MoS₂ FET without and with the h-BN layer measured in vacuum ($\sim 10^{-4}$ Torr) at room temperature. The mobility for the MoS₂ FET without the h-BN layer (figure 5(a)) and with the h-BN layer (figure 5(b)) was determined to be ~46.0 cm² V⁻¹ \cdot s⁻¹ and 52.7 cm² V⁻¹ \cdot s⁻¹, respectively. Here, a dielectric constant of 3.5 was used for the h-BN layer for the estimation of mobility values [4]. Note that the mobility of the MoS₂ FET with the h-BN layer showed a higher value than those of all the MoS₂ FETs without the h-BN layer (ranging from $0.5 \text{ cm}^2 \text{ V}^{-1} \cdot \text{s}^{-1}$ to $46.0 \text{ cm}^2 \text{ V}^{-1} \cdot \text{s}^{-1}$) characterized in this work. More importantly, hysteresis was not observed in the MoS₂ FET with the h-BN layer in contrast with the MoS₂ FETs without the h-BN layer because the h-BN layer forms a nearly ideal interface without dangling bonds and trap sites, as shown in figure 5(d). Note that in the hysteresis comparison between the two devices, we did not apply the same $V_{\rm DS}$ (figures 5(c) and (d)), but the charge trapping process is dominantly affected by V_{GS} rather than V_{DS} in our device because the electric field by $V_{\rm GS}$ is much stronger than that by $V_{\rm DS}$. Therefore, the electrical characteristics did not change in the MoS₂ FETs with the h-BN layer regardless of whether $V_{GS,before} = 40$ V or -40 V (figure 5(f)), whereas the electrical characteristics changed for $V_{GS,before} = 40$ V compared to that for $V_{GS,before} = -40$ V for the MoS₂ FETs without the h-BN layer (figure 5(e)). These phenomena can be explained in detail with the schematic diagrams in the supplementary information (figure S7). For these reasons, inserting the h-BN layer between SiO₂ and MoS₂ is desirable for realizing the stable electrical characteristics in MoS₂ FETs.

3. Conclusions

In summary, we studied the influence of a lateral electric field on the charge trapping and detrapping dynamics at the interface between the MoS_2 and SiO_2 layers. From the results of multiple V_{DS} sweeps with increasing measurement ranges of the V_{DS} , it was found that the saturation current initially decreased in the low V_{DS} sweep range and then started to increase with a larger V_{DS} sweep range over 110 V. We demonstrated that this phenomenon was due to the charge trapping and detrapping processes originating from the imperfect interface between the MoS_2 and SiO_2 dielectric. In addition, we inserted an h-BN buffer layer between MoS_2 and SiO_2 to investigate the charge trapping effect after forming a near-ideal interface. Consequently, the hysteresis caused by





trapped charges at the interface disappeared, and the trapped charge effect on electrical characteristics by $V_{GS,before}$ was also eliminated. This study provides a better understanding of the effect of interface-trapped carriers and controlling electrical characteristics by the lateral electric field in 2D material-based transistors.

4. Experimental details

4.1. Fabrication of MoS₂ FETs without and with an h-BN layer

 MoS_2 films were transferred from a bulk MoS_2 crystal on a 270 nm-thick SiO_2/Si substrate by a mechanical exfoliation method. The electron resistor layer (poly(methyl-methacrylate) (PMMA) 950 K 11% concentration in anisole) was spin-coated at 4000 rpm and then it was annealed at 180 °C for 90 s on a hot plate for the preparation of electron beam lithography. An electron beam lithography system (JSM-6510, JEOL) was used for the drain and source patterns. Ti (5 nm) and Au (30 nm) were deposited using an electron beam evaporator (KVE-2004L, Korea Vacuum Tech.) sequentially.

To fabricate the MoS_2 FET with the h-BN layer, a micro-manipulator system (AP-4200GP, UNITEK) was used for transferring MoS_2 film on the h-BN layer. After transferring MoS_2 film on the h-BN layer, it was annealed at 120 °C for 30 m on a hot plate to remove water and oxygen molecules at the interface between MoS_2 and the h-BN layer. Next, an electron beam lithography system and an electron beam evaporator system were used for the formation of the source and drain electrodes as above.



4.2. Electrical characterization

The electrical properties of the MoS₂ FETs were measured using a semiconductor parameter analyzer (Keithley 4200-SCS) at various temperatures. Raman spectra of MoS₂ were characterized using an XperRam 200 (Nanobase, Inc.) instrument with a 532 nm laser as the excitation source.

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