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Effect of Dielectric Interface on the Performance of MoS₂ Transistors

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ABSTRACT:

Due to their wide bandgap and ultrathin body properties, two-dimensional (2D) materials are currently being pursued for next-generation electronic and optoelectronic applications. While there has been increasing studies to improve the performance of MoS₂ field-effect transistors (FETs) using various methods, dielectric interface which plays a decisive role in determining the mobility, interface traps, and thermal transport of MoS₂ FETs has not been well explored and understood. In this paper, we present a comprehensive experimental study on the effect of high-*k* dielectrics on the performance of few-layer MoS₂ FETs from 300 to 4.3 K. Results show that the Al₂O₃/HfO₂ could boost the mobility and drain current. Meanwhile, MoS₂ transistors with Al₂O₃/HfO₂ afford a 2x reduction in oxide trap density compared to the devices with the conventional SiO₂ substrate. Also, we observe a negative differential resistance effect on the device with 1 μm channel length when using conventional SiO₂ as gate dielectric due to self-heating, and is being effectively eliminated by using the Al₂O₃/HfO₂ gate dielectric. This dielectric engineering provides a highly viable route to realizing high performance TMD-based FETs.

KEYWORDS: MoS₂, field-effect transistors, high *k*, pulse IV, low-frequency noise, negative differential resistance

INTRODUCTION

After decades of ongoing progress, the silicon CMOS industry is approaching a stall in device performance for logic devices due to fundamental scaling limitations. To energize the future roadmap and enable continued dimensional scaling, novel materials with unique properties are being proposed to replace silicon substrate for lower supply voltage. Recently the rich family of transition metal dichalcogenides (TMDs) MX_2 , where M stands for a transition metal (Mo, W, Nb, Ta) and X for a chalcogenide atom (S, Se, Te), have received a lot of attention for their interesting properties¹⁻⁷. Among them, molybdenum disulfide (MoS_2) is a representative semiconducting and has displayed interesting electrical, mechanical and optical properties due to a tunable bandgap of 1.2-1.8 eV and a reasonable mobility from 10-200 $\text{cm}^2/\text{V}\cdot\text{s}$ at room temperature⁸⁻¹⁷. Meanwhile, MoS_2 exhibits good thermal stability and could be grown by chemical vapor deposition in wafer-scale, providing the potential compatibility to silicon CMOS process¹⁸⁻²¹. Although great progress has been made in this field, challenges still remain to achieve high-performance MoS_2 transistors. The mobility of MoS_2 is still far below the theoretically predicted value, which is mainly limited by charged impurities and phonon scattering²². Studies have shown that the impurities and dielectric environment have an important impact on the electrical and optical properties of two-dimensional (2D) materials^{23,24}. It is reported that hexagonal boron nitride (*h*-BN) is a promising dielectric material for MoS_2 , which can significantly reduce charge traps and greatly enhance the electron field-effect mobility²⁵. However, the BN flakes are irregularly shaped and are just a few tens of micrometers long, which is a roadblock to their practical use. It has been demonstrated that utilization of high-*k* dielectric materials as the gate insulator could partially screen charged impurities and improve carrier mobility⁸. Although much work has been devoted to study the interface between high-*k*/TMDs, most of them focus on the improvement in the transport properties such as mobility²⁶⁻³¹. On the other hand, thermal conductivity (κ) of MoS_2 is very low and excessive heating can lead to poor device performance and

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3 decreased lifetimes³². Using a high thermal conductivity material as the substrate could facilitate heat
4 dissipation and relieve the self-heating effect³³. In this work, we fabricated a dual-gated MoS₂
5 transistor to make a fair comparison for the back interface with SiO₂ and the top with Al₂O₃/HfO₂.
6 Carrier transport, pulse *IV*, and low-frequency noise were comprehensively performed to investigate
7 the effect of dielectric interface on the performance of MoS₂ transistors. Results show that, compared
8 to the SiO₂ substrate, the Al₂O₃/HfO₂ could enhance the mobility and improve drain current as well
9 as more effectively eliminate the self-heating effect. Our experimental work demonstrates a
10 promising approach to improve the performance of MoS₂ transistors through substrate engineering.
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24 RESULTS AND DISCUSSION

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27 We start from mechanical exfoliation from commercially available bulk crystals. Figure 1a, b show
28 the schematic of the MoS₂ device before and after atomic layer deposition (ALD), respectively. We
29 deposited Al₂O₃ at 75 °C to avoid pinholes and nonuniformity in the film. The thickness of MoS₂
30 used in this work is 4.2 nm, as shown in the inset of Fig. 1c, measured by atomic force microscopy
31 (AFM). The channel length and width of the MoS₂ transistor are 1 and 4.2 μm, respectively. All the
32 measurements were carried out under vacuum (< 10⁻⁵ Torr) in a Lakeshore cryogenic probe station
33 using an Agilent parameter analyzer B1500A. The low-frequency 1/*f* noise measurements were
34 carried out by Agilent B1500A and E5052B with a resistor unit.
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49 We first study the effect of Al₂O₃/HfO₂ capping on the electrical properties of MoS₂ transistors.
50 Figure 2a shows the *I_d-V_g* curves of back-gate MoS₂ before and after Al₂O₃/HfO₂ deposition. As
51 shown in the inset of Fig. 2a, it is clear that the threshold voltage *V_{th}* shifts toward negative values of
52 around 6 V due to the doping of Al₂O₃/HfO₂^{27,28}, suggesting a doping density of 1.4 × 10¹² cm⁻².
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3 Figure 2b shows the transfer characteristics of the back-gate and top-gate MoS₂ transistors at $V_d =$
4 0.05 V. The threshold voltage of back-gate and top-gate FETs are -17.5 and -15.6 V, respectively.
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6 The negative V_{th} is mainly due to the doping effect from Al₂O₃/HfO₂. A well-behaved output
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8 characteristic of a 1 μm -channel-length MoS₂ transistor with 90 nm SiO₂ gate dielectric is
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10 demonstrated in Fig. 2c, exhibiting a maximum drain current of 188 $\mu\text{A}/\mu\text{m}$ with $V_d = 3$ V and $V_{bg} =$
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12 40 V at 300 K. For the top gate with Al₂O₃/HfO₂ gate dielectric, the maximum drain current is 290
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14 $\mu\text{A}/\mu\text{m}$ with $V_d = 3$ V and $V_{tg} = 10$ V when fixed $V_{bg} = 0$ V. The on-current drivability of the top
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16 device is higher than the back device with SiO₂ gate dielectric due to better interface quality as well
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18 as a high mobility. Figure 2e shows a comparison of drain current for back gate and top gate at
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20 various temperatures. It is clear that at all temperature the drain current of the top gate is larger than
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22 that of the back gate, indicating that high k dielectric is more effective to improve the performance of
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24 MoS₂ transistors. Figure 2f compares peak transconductance (g_m) for the back-gate and the top-gate
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26 MoS₂ transistors at $V_d = 0.05$ V from 300 to 20 K. The g_m increases with decreasing temperature for
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28 both devices. As expected at all temperatures, the g_m is always higher for the top-gate device. The
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30 field-effect mobility μ_{FE} is extracted in the linear region of the transfer characteristics according to
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32 the following equations $\mu_{FE} = g_m / (C_g EW)$ and $(E = (V_d - 2R_c I_d) / L)$, where g_m is the
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34 transconductance, C_g is the gate capacitance, E is the transverse electric field in the channel, L and W
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36 are the length and width of the channel, respectively, I_d is the drain current, and R_c is the contact
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38 resistance¹². The mobility of the SiO₂ and Al₂O₃/HfO₂ devices at 300 K are 55 and 81 $\text{cm}^2/\text{V}\cdot\text{s}$,
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40 respectively. This improvement in mobility could be attributed to the reduction of Coulomb
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42 scattering by dielectric screening²⁵, which implies that Al₂O₃/HfO₂ dielectric has greater potential to
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44 realize high-performance transistors with TMDS channel materials.
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3 It is well known that conventional DC characterization methods have charge trapping phenomena
4 that occur during long measurements³⁴. To minimize the effect of charge trapping and de-trapping,
5 pulsed I_V measurement is required to obtain the intrinsic electrical characteristics of the MoS₂
6 transistors^{35,36}. DC I_d is compared with I_d measured using different pulse widths, as V_d is swept from
7 0 to 3.5 V with $V_{bg} = -30$ V at 300 K as shown in Fig. 3a. The pulse width is changed from 5 ms
8 (blue) to 25 ms (magenta). At all V_{tg} , the drain current increases with shorter pulse width and the DC
9 measurement has the lowest drain current. With increasing V_{bg} to 0 V, the corresponding I_d - V_d curves
10 are shown in Fig. 3b. Similar to the case in (a), all the pulsed curves are higher than the DC curves.
11 The more traps in the interface, the much drain current degradation ΔI_d ³⁶. To investigate the interface
12 quality, we define that ΔI_d is the difference between the DC and the pulse measurements with 5 ms
13 pulse width at $V_d = 2$ V. Figure 3c shows ΔI_d versus V_{bg} with various V_{tg} at 300 K. It is apparent that
14 ΔI_d increases with increasing V_{bg} and the trend is independent of V_{tg} . Owing to the intrinsic n-type of
15 MoS₂, electrons in the MoS₂ channel will be close to Al₂O₃/MoS₂ interface when the V_{bg} is negative
16 and will move to near the SiO₂/MoS₂ interface for positive V_{bg} . ΔI_d is proportional to the magnitude
17 of traps³⁶. Hence, the change in ΔI_d shows that there are fewer traps in the Al₂O₃/MoS₂ interface
18 indicating a better interface quality compared to SiO₂/MoS₂ interface. Figure 3d shows ΔI_d as a
19 function of V_{tg} with different V_{bg} at 300 K for the same two devices in (c). Obviously, ΔI_d decreases
20 with increasing V_{tg} irrespectively of V_{bg} . The explanation is similar to that in (c). For $V_{tg} < 0$ V,
21 electrons accumulate near to the SiO₂/MoS₂ interface. For $V_{tg} > 0$ V, electrons approach to the
22 Al₂O₃/MoS₂ interface. This result also shows that interface quality of Al₂O₃/MoS₂ is better than that
23 of SiO₂/MoS₂.
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53 Low-frequency $1/f$ noise is also important which limits the performance of electronic communication
54 systems and sensors³⁷. For example, low-frequency noise determines noise-to-signal ration in digital
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3 electronic device and low-frequency noise can be upconverted to phase noise in oscillators³⁸. Here,
4 we performed the low-frequency noise measurement on the back-gate MoS₂ device and the top-
5 gate MoS₂ device in the linear region with $V_d = 0.2$ V at 300 K. The noise spectra can be
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8 quantitatively characterized by $S_{id} = \frac{AI_d^2}{f^\gamma}$, where S_{id} is the current noise power spectral density, f is
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11 the frequency, I_d is the current through the device channel, γ is frequency exponent, and A is the noise
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14 amplitude^{39,40}. We extract the noise amplitude A using

$$15 \quad A = (1/N) \sum_{m=1}^N f_m S_{Im} / I_m^2 \quad (1)$$

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18 where S_{Im} and I_m are the noise spectral density and drain current measured at m different
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21 frequencies⁴¹. Figure 4a shows the normalized A of the back-gate and top-gate MoS₂ transistors as a
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24 function of carrier density at 300 K. The noise amplitude from the top gate improves more than 40%
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27 than that from the back gate for the same carrier density, indicating that the interface quality of
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30 Al₂O₃/MoS₂ is better than that of the SiO₂/MoS₂. To evaluate quantitatively the interface property,
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33 we estimate the oxide trap density (N_{ot}) using input-referred voltage noise spectral density S_{vg} at the
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36 threshold voltage (V_{th}) as shown in Fig. 4b. It can be seen that the top-gate exhibits a reduced noise,
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39 implying a lower oxide trap density. The previous studies have demonstrated that the dominant noise
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42 mechanism of few-layer MoS₂ transistor is number carrier fluctuation^{12,42,43}. It is then possible to
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45 evaluate the oxide trap density using the following formula^{44,45}:

$$46 \quad S_{vg} = \frac{N_{ot} k T q^2}{\alpha f W L C_g^2} \quad (2)$$

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49 where q is the element charge, kT is the thermal energy, and α is the tunneling constant ($\alpha = 10^8$ cm⁻¹
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52 is used here). The trap depth z at which the traps in the oxide is measured is derived from the
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55 noise frequency using⁴⁶:

$$z = \frac{1}{\alpha} \ln \frac{1}{2\pi f \tau_0} \quad (3)$$

where the time constant τ_0 is often taken as 10^{-10} s. Based on Eqs (2) and (3), we extracted the oxide trap density profile for the back-gate and top-gate transistors. The depth z of both devices is 1.43-1.90 nm with the noise measurements in the frequency ranging from 10 to 1000 Hz. Figure 4c shows the oxide trap density as a function of depth for both devices. The N_{ot} of $7.7 \times 10^{19} - 1.1 \times 10^{20} \text{ cm}^{-3} \text{ eV}^{-1}$ for the top-gate device is lower than that of the back-gate device (i.e., $1.2 \times 10^{20} - 2.0 \times 10^{20} \text{ cm}^{-3} \text{ eV}^{-1}$). This result is well agreement on our observation from pulse IV and consistent with the previous reports^{47,48}.

To further demonstrate the advantage of $\text{Al}_2\text{O}_3/\text{HfO}_2$, we compare the output characteristic of the back-gate and top-gate MoS_2 transistors at 70 and 4.3 K. Figure 5a depicts the well-behaved output characteristic of the back-gate device using SiO_2 substrate with V_d sweeping from 0 to 4 V for four different V_{bg} at 70 K. At $V_{bg} = 25$ V, the maximum drain current is $375 \mu\text{A}/\mu\text{m}$ and the curve exhibits current saturation. With increasing V_{bg} further, the drain current increases accordingly and even shows the sign of negative differential resistance (NDR) effect when I_d is larger than $400 \mu\text{A}/\mu\text{m}$ due to self-heating effect, which is consistent with the previous studies^{12, 49}. The saturation current degradation $\Delta I/I_{sat}$ with $V_{bg} = 40$ V at 70 K is 1.2%. This is predictable since both of MoS_2 and SiO_2 have a low thermal conductivity indicating a poor heat transport behavior^{32,33}. The local heating of MoS_2 - SiO_2 interfaces could be even more pronounced compared to that of Si - SiO_2 interfaces in modern SOI (silicon-on-insulator) structures, which could be an important issue for high-performance MoS_2 transistors with scaling⁵⁰. For efficient heat dissipation from MoS_2 channel, substrates with high thermal conductivity (κ) are desirable, e.g., Al_2O_3 ($\kappa = 35 \text{ W/m}\cdot\text{K}$), instead of commonly used SiO_2 ($\kappa = 1.4 \text{ W/m}\cdot\text{K}$)³³. Figure 5b shows the output characteristic of the top-gate

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3 MoS₂ transistors at 70 K with top-gate biases V_{tg} range from 4 to 10 V with a 2 V step and V_{bg} fixed
4 at 0 V. We didn't observe any NDR effect even 18% improvement in drain current over the sample
5 in (a), indicating an efficient heat dissipation using high thermal conductivity Al₂O₃. With increasing
6 V_{bg} to 40 V, the drain current is over 600 $\mu\text{A}/\mu\text{m}$ without NDR effect as shown in Fig. 5c. When
7 decreasing the temperature down to 4.3 K, the drain current increases accordingly as shown in Fig.
8 5d-f. The saturation current degradation $\Delta I/I_{sat}$ of the back-gate device with $V_{bg} = 40$ V at 4.3 K is
9 1.6% as shown in Figure 5d, which is larger than that of 1.2% at 70 K in (a). This confirms that the
10 NDR effect is more pronounced in higher drain current due to self-heating effect⁵¹. At $V_{bg} = 40$ V and
11 4.3 K, the drain current of the top-gate device is larger than 620 $\mu\text{A}/\mu\text{m}$ as shown in Figure 5f, up to
12 660 $\mu\text{A}/\mu\text{m}$ at $V_{tg} = 10$ V. When the drain current is greater than 635 $\mu\text{A}/\mu\text{m}$, we observed the sign of
13 NDR effect again. The $\Delta I/I_{sat}$ with $V_{tg} = 10$ V and $V_{bg} = 40$ V at 4.3 K is 0.5%, which is three times
14 smaller than that in (d). This result shows that Al₂O₃/HfO₂ is more efficient to remove self-heating. It
15 should be noted that the NDR is strongly related with the width and channel length of MoS₂
16 transistors, which determines the area of dissipation during device operation. With further scaling,
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42 CONCLUSIONS

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45 In conclusion, we report a high-performance MoS₂ transistor. We systematically compare the effect
46 of Al₂O₃/HfO₂ and SiO₂ substrates on the mobility, drain current, oxide trap density, and NDR of
47 MoS₂ devices. Benefiting from the high dielectric constant and high thermal conductivity of
48 Al₂O₃/HfO₂, the MoS₂ transistor with Al₂O₃/HfO₂ exhibits a high mobility of 81 cm²/V·s and less
49 oxide trap density. The maximum drain current of the top-gate device with a 1 μm -channel-length is
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up to 660 $\mu\text{A}/\mu\text{m}$ at 4.3 K. Meanwhile, $\text{Al}_2\text{O}_3/\text{HfO}_2$ substrate reduces the self-heating effect. Our work provides a viable path to improve the device performance of TMD-based FETs.

METHODS

By standard scotch-tape techniques, few-layer MoS_2 were transferred to heavily doped silicon substrate which was capped with 90 nm SiO_2 . Then it soaked in undiluted 1, 2 dichloroethane (DCE) at room temperature for more than 12 h. Source/drain regions were defined by e-beam lithography, followed by a Ni/Au metallization of 15/45 nm with e-beam evaporator. The gap between source and drain was 1 μm . After the device was first measured with back gate only, the top gate dielectric was grown by ALD. First, a 25 nm Al_2O_3 was deposited with trimethylaluminum and H_2O as precursors at 75 $^\circ\text{C}$ and then 20 nm HfO_2 was in situ deposited using tetradimethylaminohafnium and H_2O as precursors at 150 $^\circ\text{C}$. The dielectric constant of Al_2O_3 and HfO_2 are 6 and 12, respectively. The top gate was defined with e-beam lithography and Ti/Au of 15/45 nm was used as the top gate. No annealing was performed during the process.

FIGURES

Figure 1. (a) Cross-section schematic view of a back-gate MoS_2 device. (b) Cross-section schematic view of a dual-gate MoS_2 device. (c) AFM images of the MoS_2 device. The MoS_2 flake is 4.2 nm measured by AFM.

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3 **Figure 2.** (a) Transfer characteristics of the back-gate MoS₂ device before and after Al₂O₃/HfO₂
4 capping at 300 K. Inset: The linear coordinated transfer curves. (b) Transfer characteristics of the
5 back-gate and top-gate MoS₂ device at 300 K. (c) Output characteristics of the back-gate MoS₂
6 device at 300 K. V_{bg} is from -40 to 40 V in 5 V step with V_d from 0 to 3 V. (d) Output characteristics
7 of the top-gate MoS₂ transistor with V_{bg} fixed at 0 V at 300 K. V_{tg} is from -16 to 10 V in 2 V step and
8 V_d from 0 to 3 V. (e) Comparison of maximum drain current of the same two devices in (c) and (d)
9 at different temperatures. (f) Comparison of g_m of the same two devices in (c) and (d) at various
10 temperatures.
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24 **Figure 3.** Output characteristics of the top-gate MoS₂ transistor at 300 K with 3 V steps in V_{tg} from -
25 10 to 8 V with comparison between DC measurement and different pulse widths (pulse width = 5, 15,
26 and 25 ms) for (a) $V_{bg} = -30$ V and (b) $V_{bg} = 0$ V. (c) ΔI_d as a function of V_{bg} for the same device in (a)
27 at various V_{tg} with $V_d = 2$ V. (d) ΔI_d as a function of V_{tg} for the same device in (a) at various V_{bg} with
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39 **Figure 4.** (a) Inverse noise amplitude $1/A$ as a function of carrier density at $V_d = 0.2$ V. (b) Input gate
40 voltage noise versus frequency for the same two devices in (a). (c) Oxide trap density versus trap
41 depth, derived from the low-frequency noise spectrum at their corresponding threshold voltage $V_{th,t}$
42 and $V_{th,b}$.
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50 **Figure 5.** (a) The output characteristics of the back-gate MoS₂ transistor at 70 K. V_{bg} is from 25 to 40
51 V with 5 V steps. The I_d - V_d characteristics of the top-gate device at 70 K with (b) $V_{bg} = 0$ V, and (c)
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3 $V_{bg} = 40$ V. V_{tg} is from 4 to 10 V with 2 V steps. (d-f) The I_d - V_d characteristics of the corresponding
4 devices in (a-c) at 4.3 K.
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10 ASSOCIATED CONTENT

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14 Notes

15 The authors declare no competing financial interest.
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Figure 1

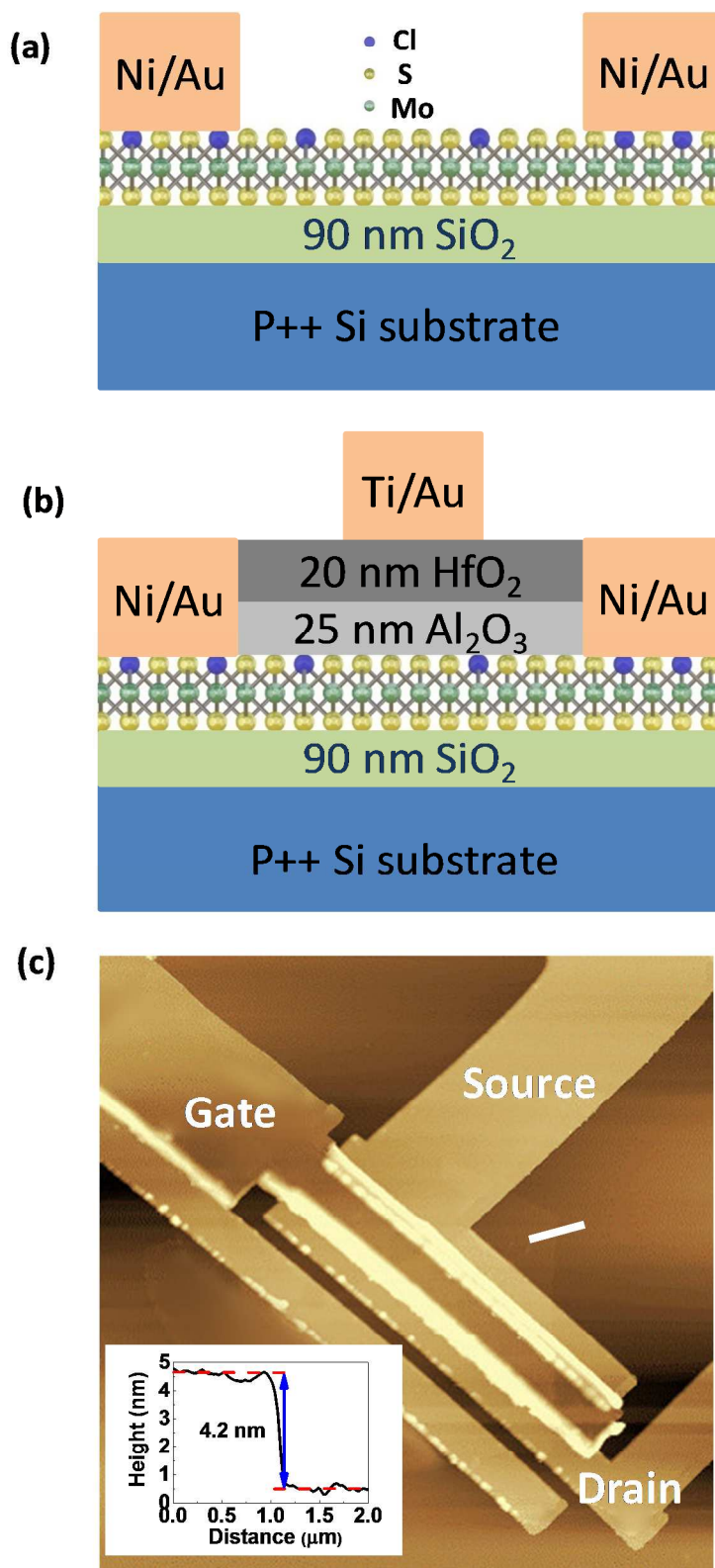


Figure 2

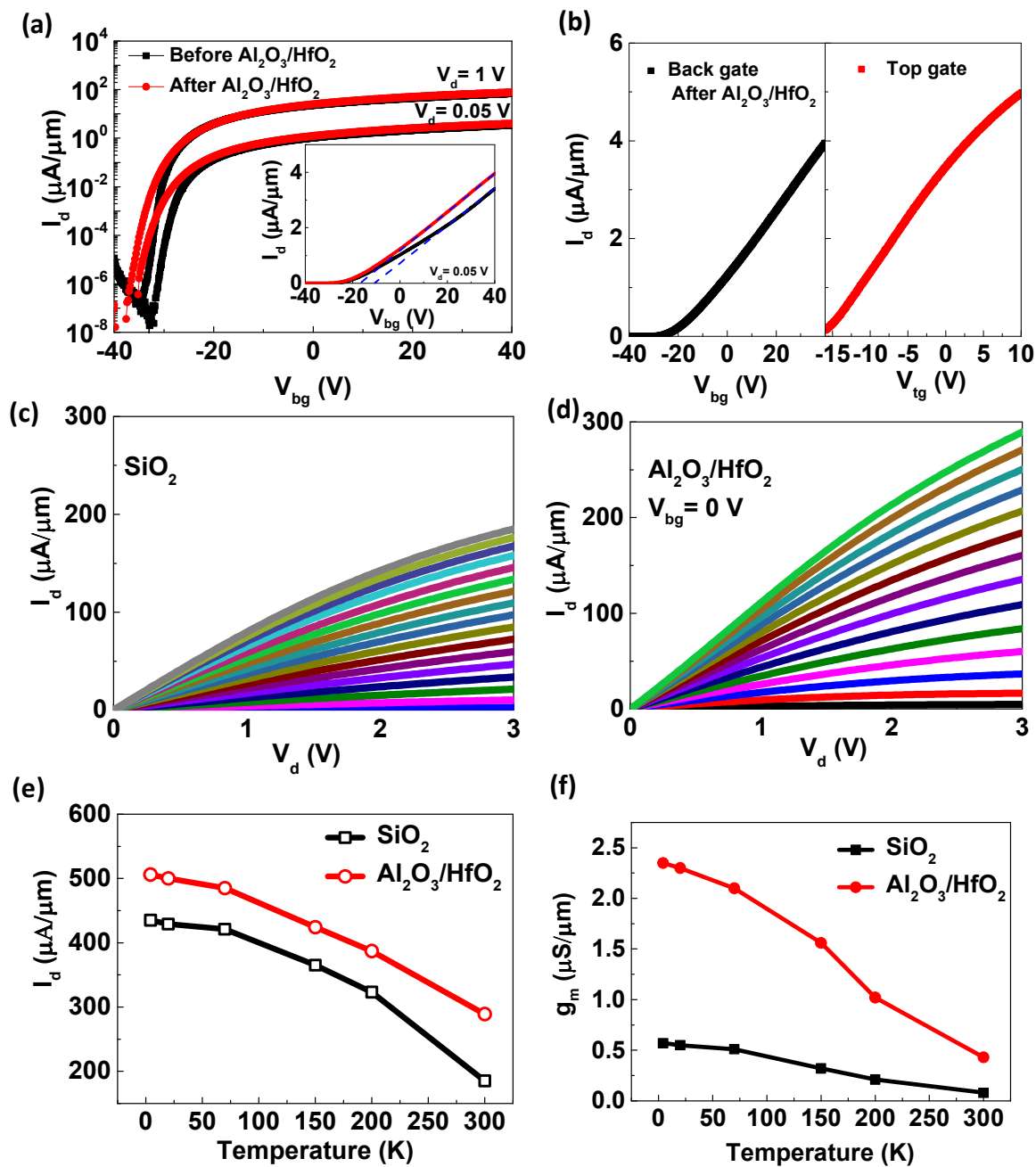


Figure 3

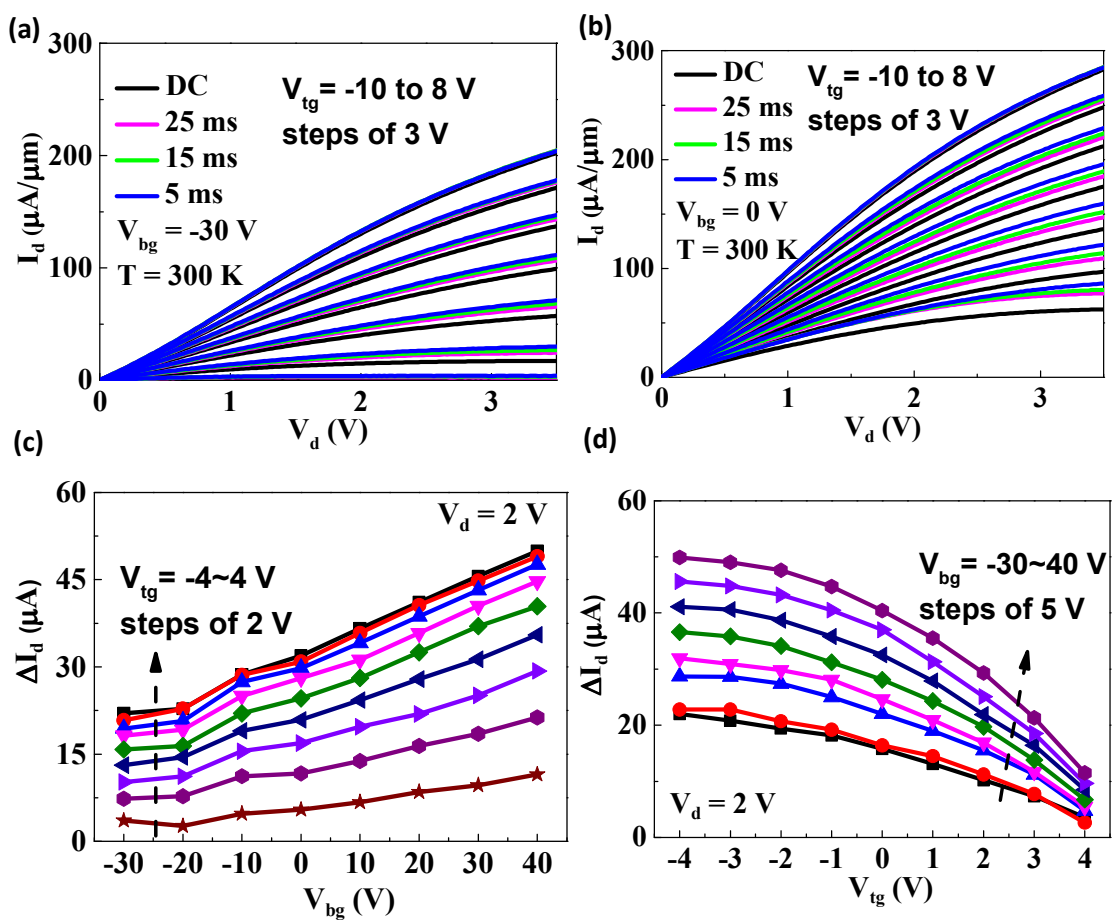


Figure 4

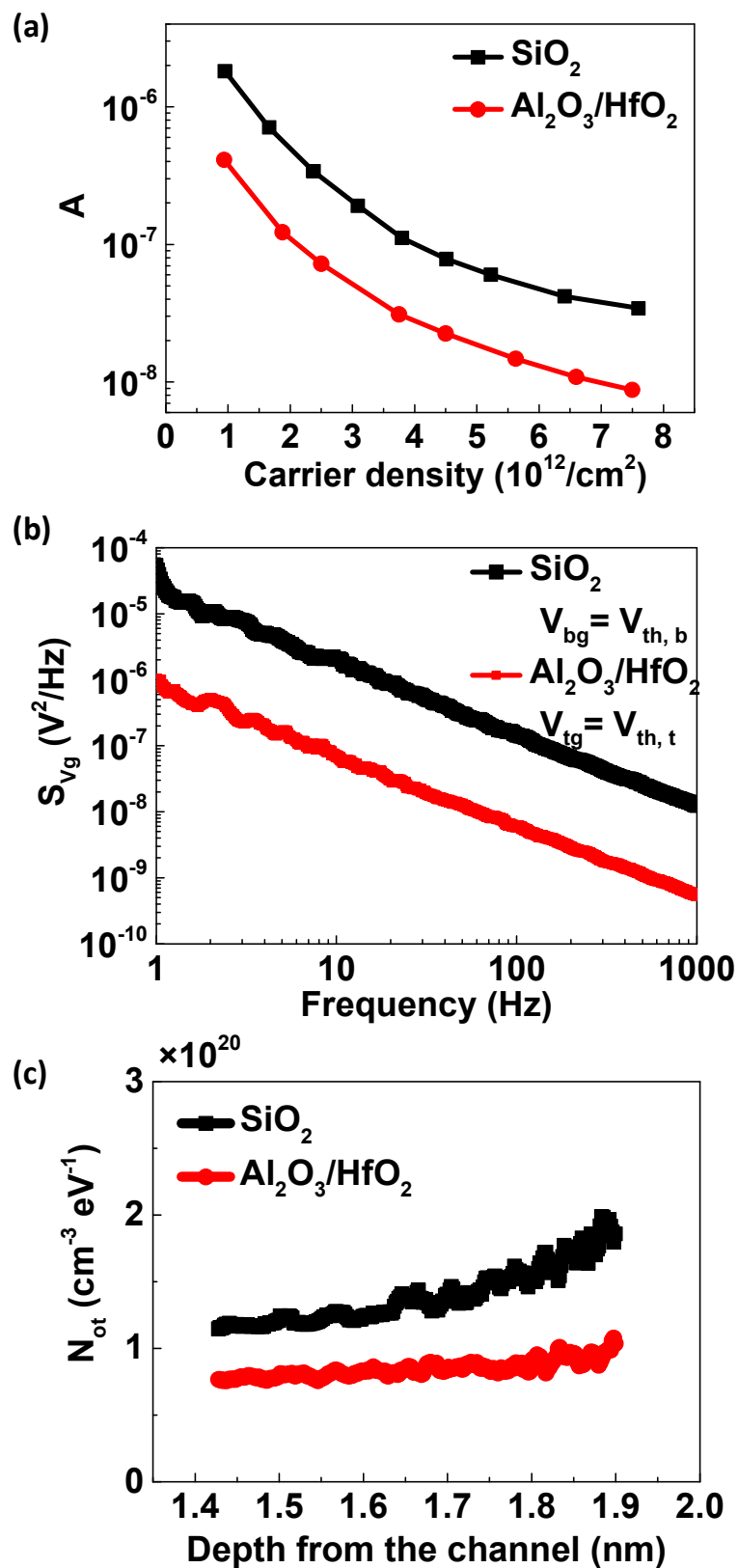


Figure 5

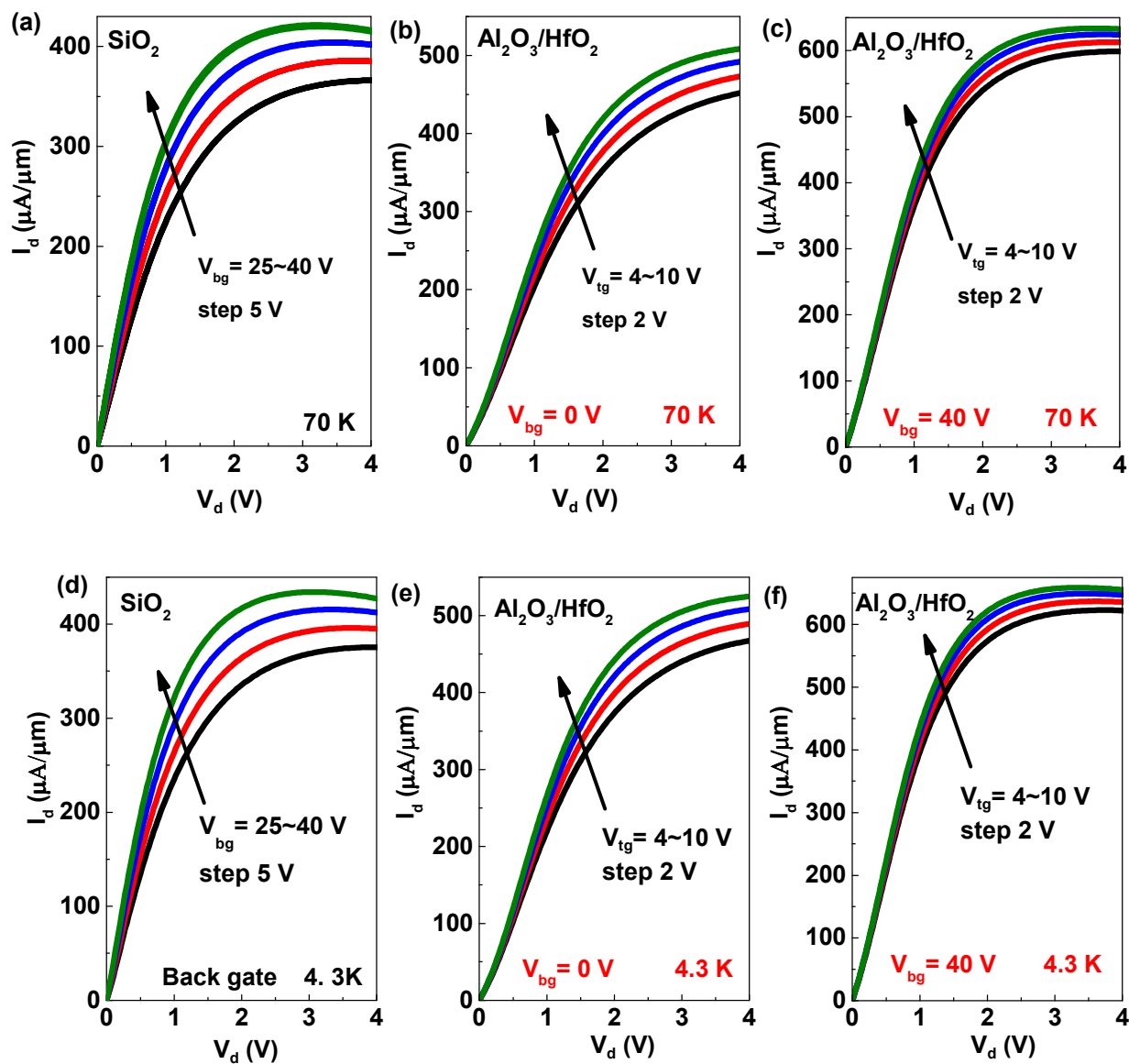


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