# ALD-ZrO<sub>2</sub> Gate Dielectric with Suppressed Interfacial Oxidation for High Performance MoS<sub>2</sub> Top Gate MOSFETs

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Abstract —To enhance the feasibility of 2D transition metal dichalcogenide channels in nano-electronic devices, a top gate device structure fabricated with Very-Large-Scale-Integration compatible process is desired. High-κ dielectric ZrO<sub>2</sub> has been directly deposited on MoS<sub>2</sub> through low temperature atomic layer deposition. Physical adsorption instead of chemical reaction was confirmed at the interface between ZrO<sub>2</sub> and MoS<sub>2</sub>, which helps to suppress interfacial oxidation and reduce damage. While scaling down capacitance equivalent thickness of ZrO<sub>2</sub>, low thermal budget post deposition annealing was effective for reducing interfacial traps, thus enhancing the device performances of monolayer MoS<sub>2</sub> nMOSFETs.

# 1. Introduction

Atomic-layer transition metal dichalcogenides (TMDCs) have attracted considerable attention owing to their promising properties for future nano-electronic applications. MoS2, a well-known TMDC channel material shows great potential in low-power-consumption device field. To fulfill the requirement of VLSI (Very-Large-Scale-Integration) applications, fabricating high performance top gate MoS<sub>2</sub> MOSFETs using chemical vapor deposition (CVD) grown MoS<sub>2</sub> with high quality gate dielectric is indispensable. However, because of the lack of surface dangling bonds, it is still very challenging to obtain high quality high-ĸ/MoS2 interface with low capacitance equivalent thickness (CET) through atomic layer deposition (ALD) approach [1,2]. Recently, we have reported uniform deposition of ZrO2 on CVD-grown MoS<sub>2</sub> by plasma enhanced ALD (PEALD) [3], which showed the decent device performance and high dielectric constant. Although high oxidation efficiency of PEALD promotes uniform layer deposition, the degradation of interfacial quality owing to MoS<sub>2</sub> oxidation was addressed. In order to further enhance device performance as well as gate control of channel, optimization of ALD processes not to damage the surface of 2D materials and CET scaling of ZrO2 are necessary.

In this work, uniform deposition of  $ZrO_2$  as gate dielectrics on CVD-grown MoS<sub>2</sub> were obtained through ALD even at low deposition temperature at 150 °C, leading to significantly suppressed interfacial oxidation. The CET scaling of  $ZrO_2$  down to 2.3 nm was also demonstrated. In addition, the top gate monolayer (1L) MoS<sub>2</sub> MOSFETs exhibited reduced subthreshold swing (SS) and improved hysteresis as the benefits of low temperature post deposition annealing (PDA) and CET scaling.

## 2. Experimental

The detailed process flow for fabricating 1L  $MoS_2$  top gate MOSFETs is shown Fig 1(a). The schematic cross-

section and top view of optical microscope photograph of  $MoS_2$  devices are shown in Fig. 1(b) and 1(c), respectively. Salt-assisted CVD was used to synthesize  $MoS_2$  directly on SiO<sub>2</sub> (285 nm)/Si substrates using  $MoO_2$  and sulfur powder. KBr was used as a growth promoter, as described previously [4]. After 1L  $MoS_2$  growth, the S/D contacts were formed with photolithography and e-beam evaporation. Then, the ZrO<sub>2</sub> gate dielectrics were deposited at 150 °C thorough ALD using TEMAZ and H<sub>2</sub>O as precursors with different deposition cycles, which denotes as LT-ALD afterwards. Finally, after 300 °C PDA in N<sub>2</sub> ambient, the top gate electrodes were deposited through e-beam evaporation. Top gate  $MoS_2$  MOSFETs with PEALD ZrO<sub>2</sub> gate dielectrics deposited at 300 °C [3] were also prepared for comparison, which denotes as HT-PEALD afterwards.



Fig. 1(a) Process flow for fabricating MoS<sub>2</sub> top gate MOSFETs, (b) schematic cross-section and (c) top view of optical microscope photograph of the fabricated devices.

#### 3. Results and Discussion

Fig. 2 shows the HR-TEM cross-sectional image of  $MoS_2$  channel with LT-ALD  $ZrO_2$  gate dielectric. The channel thickness of 0.7 nm, corresponding to 1L  $MoS_2$ , is clearly seen with the abrupt  $ZrO_2/MoS_2$  interface.



Fig. 2 HR-TEM cross-sectional images of 1L  $MoS_2$  channel with ALD-ZrO\_2 gate dielectric.

Fig. 3(a) shows Mo 3d XPS spectra extracted from 2nm-thick ZrO<sub>2</sub> on bulk MoS<sub>2</sub>, which was mechanically exfoliated from MoS<sub>2</sub> flakes. The spectrum extracted from pristine MoS<sub>2</sub> flakes was also shown for comparison. The Mo 3d spectra for pristine and LT-ALD samples show similar feature with three peaks, which are attributed to the doublet of Mo<sup>4+</sup> 3d<sub>3/2</sub> and Mo<sup>4+</sup> 3d<sub>5/2</sub> and S<sup>2-</sup> 2s states in MoS<sub>2</sub>. This indicates the ZrO<sub>2</sub> deposition at 150 °C mainly results from physical absorption instead of chemical reaction between ZrO<sub>2</sub> and MoS<sub>2</sub>. On the other hand, additional Mo<sup>6+</sup> 3d<sub>3/2</sub> and Mo<sup>6+</sup> 3d<sub>5/2</sub> states, correlating to MoO<sub>3</sub> were observed in HT-PEALD samples. This suggests the existence of Mo oxide interfacial layer owing to high oxidation efficiency of high temperature PEALD, which also explain the difficulty in obtaining device operation of 1L MoS<sub>2</sub> devices with PEALD ZrO<sub>2</sub> gate dielectrics [3]. Meanwhile, no obvious difference was observed in S 2p XPS spectra as shown in Fig. 3(b), which exhibited two peaks resulting from the doublet of S<sup>2-</sup> 2p<sub>1/2</sub> and S<sup>2-</sup> 2p<sub>3/2</sub> states in MoS<sub>2</sub>. All these peaks are consistent with the reported values for MoS<sub>2</sub> crystal.



Fig. 3(a) Mo 3d and (b) S 2p XPS spectra extracted from HT-PEALD  $ZrO_2/MoS_2$ , LT-ALD  $ZrO_2/MoS_2$  and pristine  $MoS_2$ , respectively.

The impact of  $ZrO_2$  deposition on the device performance of MoS<sub>2</sub>/SiO<sub>2</sub> back gate transistors was investigated. Fig. 4 shows the  $I_D$ - $V_G$  transfer curves extracted from MoS<sub>2</sub> MOSFETs under back gate operation before and after ZrO<sub>2</sub> deposition on top of the MoS<sub>2</sub> surface. Even with 2-layer (2L) MoS<sub>2</sub> channel, those devices with HT-PEALD ZrO<sub>2</sub> demonstrate degraded features in terms of lower on-state current and worse SS after ZrO<sub>2</sub> deposition. On the other hand, no obvious degradation was found in LT-ALD 1L MoS<sub>2</sub> case, indicating the benefits of low temperature ALD process to suppress damages due to oxidation of MoS<sub>2</sub> surface. Less damage of MoS<sub>2</sub> channel with no interfacial layer is consistent with the result in Fig. 2.



Fig. 4  $I_{D}$ - $V_G$  transfer curves extracted from MoS<sub>2</sub> MOSFETs under back gate operation before and after (a) HT-PEALD and (b) LT-ALD ZrO<sub>2</sub> encapsulation on top of MoS<sub>2</sub> surface.

To understand the influence of low thermal budget PDA, Fig. 5 (a) shows the  $I_D$ - $V_G$  characteristics of 5 µm-gatelength 1L MoS<sub>2</sub> MOSFETs under top gate operation measured before and after 300 °C PDA. Normal nMOSFETs operation behaviour was clearly observed with a high on-off ratio of 10<sup>7</sup> after PDA. It was found the low thermal budget PDA is effective for reducing interfacial traps, since the SS drastically decrease from ~170 to ~90 mV/decade after PDA as shown in Fig. 5(b). As the scattering factor suppressed, enhanced on-state current was also obtained. (Fig. 5(a)) Besides, the drain induced barrier lowering (DIBL) was also significantly reduced, which may be attributed to the improvement of contact resistance after PDA.



Fig. 5 (a)  $I_D$ - $V_G$  characteristics of 5 µm-gate-length 1L MoS<sub>2</sub> top gate MOSFETs measured before and after 300 °C PDA and (b) The  $I_D$  dependence of extracted SS.

The CET scaling effect on device performance was also characterized. Fig. 6(a) shows the split-CV curves at frequency of 10 kHz extracted from MoS<sub>2</sub> nMOSFETs with ZrO<sub>2</sub> deposited with ALD 50 and 100 cycles. Based on maximum C<sub>ox</sub>, the CET was determined to be 2.3 and 4.4 nm. The dielectric constant of ZrO<sub>2</sub> was calculated to be 13.4 by using ZrO<sub>2</sub> physical thickness, which was relatively lower than that of HT-PEALD samples [3]. The deposition temperature induced phase transition may explain this phenomenon, and this can be avoided by optimizing ALD conditions and/or PDA. Fig. 6(b) shows gate hysteresis curves for 1L MoS<sub>2</sub> devices with different CET. Decent device performance maintained with CET shrinking down to 2.3 nm. Higher on-state current with reduced gate hysteresis, indicating the benefits of CET scaling.



Fig. 6(a) Split-CV characteristics at frequency of 10 kHz and (b)  $I_{\rm D}$ - $V_{\rm G}$  hysteresis curves at  $V_{\rm D}$  of 1 V extracted from 1L MoS<sub>2</sub> devices with different ALD growth cycles.

### 4. Conclusion

1L MoS<sub>2</sub> top gate MOSFETs using ALD ZrO<sub>2</sub> gate dielectrics has been demonstrated with VLSI-compatible gate stack formation processes. Low ALD deposition temperature promotes physical adsorption, leading to significantly suppressed surface oxidation and less damaged MoS<sub>2</sub> channel. Decent operation behavior maintained while ZrO<sub>2</sub> CET scaling down to 2.3 nm, indicating the low thermal budget process is beneficial for MoS<sub>2</sub> channel. Further CET scaling would be expected by ZrO<sub>2</sub> thickness scaling.

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