### **Supporting Information**

## Suppression of Surface Optical Phonon Scattering by AlN Interfacial Layers for Mobility Enhancement in MoS<sub>2</sub> FETs

Woonggi Hong,<sup>1</sup> Gi Woong Shim,<sup>2</sup> Hyeok Jun Jin,<sup>2</sup> Hamin Park,<sup>3</sup> Mingu Kang,<sup>2</sup> Sang Yoon Yang,<sup>2</sup> and Sung-Yool Choi<sup>2,\*</sup>

<sup>1</sup> School of Electronics and Electrical Engineering, Convergence Semiconductor Research Center, Dankook University,
 152 Jukjeon-ro, Suji-gu, Yongin-si, Gyeonggi-do 16890, Republic of Korea

<sup>2</sup> School of Electrical Engineering, Graduate School of Semiconductor Technology, Korea Advanced Institute of Science and Technology (KAIST), 291 Daehak-ro, Yuseong-gu, Daejeon 34141, Republic of Korea

<sup>3</sup> Department of Electronic Engineering, Kwangwoon University, 20 Gwangun-ro, Nowon-gu, Seoul 01897, Republic of Korea

\*E-mail: sungyool.choi@kaist.ac.kr

#### Figure S1: MOCVD-grown MoS<sub>2</sub> thin film



**Figure S1.** (a) Photograph of the  $MoS_2$  thin film grown on a SiO<sub>2</sub>/Si substrate. (b) Optical microscopy (OM) image and (c) scanning electron microscopy (SEM) image of metal-organic chemical vapor deposition (MOCVD)-grown  $MoS_2$  thin film.





**Figure S2.** XPS spectra of (a) N 1s and (b) Mo 3d in AlN/MoS<sub>2</sub> stack corresponding to the plasma power for AlN deposition.

#### Figure S3: XPS analysis for AlN film



**Figure S3.** (a) AlN deposited on SiO<sub>2</sub> and the XPS spectrum with (b) N 1s showing N-C bond and (c) C 1s showing C-N bond.

#### Figure S4: MoS<sub>2</sub> FETs images



Figure S4. (a) OM image of  $MoS_2$  FETs with bottom gate-staggered structure and (b) its magnified image.



Figure S5: TEM analysis for MoS<sub>2</sub> thin film sandwiched by AlN interfacial layers

**Figure S5.** (a) Cross-sectional TEM image of  $MoS_2$  thin film sandwiched by AlN interfacial layers and (b) its Energy-dispersive X-ray spectroscopy mapping image. (c) Elemental distributions along the scan direction in (a). (d) Elemental distribution around  $MoS_2$  thin film and (e) its corresponding stacking structure.





Figure S6. (a) Energy band diagram of  $MoS_2$  before and after the bandgap reduction by conduction band edge. (b) Schottky barrier height change after the bandgap reduction resulting from strain.

# Figure S7, S8, and S9: Electrical characteristics of MoS<sub>2</sub> FETs according to the interface types

Compared with MoS<sub>2</sub> FETs with Al<sub>2</sub>O<sub>3</sub> sandwich structure, MoS<sub>2</sub> FETs with AlN TIL (regardless of the BIL types) yield off-current level increases due to the lowering of the Schottky barrier height by strain,<sup>1-3</sup> resulting in the degradations in terms of on/off current ratio and SS, as shown in Figure S9a. As a result of SS change,  $V_T$  extracted from 10<sup>-7</sup> A by the constant current method varies accordingly.<sup>4</sup> When MoS<sub>2</sub> FETs use AlN as the TIL (regardless of the BIL types), the strain effect caused by incorporating nitrogen atoms into the MoS<sub>2</sub> thin film remains similar, resulting in comparable  $V_T$  values. However, MoS<sub>2</sub> FETs with AlN BIL also yield negative shift trends in  $V_T$  compared with the MoS<sub>2</sub> FETs with Al<sub>2</sub>O<sub>3</sub> sandwich structure. It is well known that the AlN/Al<sub>2</sub>O<sub>3</sub> gate dielectric stack demonstrates an excellent interface quality with MoS<sub>2</sub> by reducing the trap density near the interface.<sup>5</sup> Therefore, a steeper slope in the subthreshold region could be achieved

by the rapid transition of the off- to the on-state, showing the negatively shifted  $V_T$ . From the  $n_{2D}$  viewpoint, using plasma for AlN deposition causes nitrogen to penetrate the MoS<sub>2</sub> thin film,<sup>6</sup> inducing strain and modifying the band structure at the MS junction, as shown in Figure S6b,<sup>1-3</sup> thereby changing the  $n_{2D}$  value. That is,  $n_{2D}$  is only affected by the types of TIL. For this reason, MoS<sub>2</sub> FETs with AlN TIL always yield higher  $n_{2D}$  values than MoS<sub>2</sub> FETs with Al<sub>2</sub>O<sub>3</sub> TIL regardless of the BIL types.



**Figure S7.** Gate leakage current characteristics of MoS<sub>2</sub> FETs in log scale according to the interface types



Figure S8. Representative output characteristics of MoS<sub>2</sub> FETs with different types of interfacial layers ranging from  $V_{GS} - V_T = 0$  V to  $V_{GS} - V_T = 4$  V (step of 1 V).



**Figure S9.** Device parameters including (a)  $I_{on}/I_{off}$ , SS, (b)  $V_T$ , and  $n_{2D}$  extracted from MoS<sub>2</sub> FETs with different interfacial layers.

# Figure S10 and S11: Electrical characteristics of graphene FETs with AIN interfacial layers

Graphene exhibits a symmetric energy band structure known as the Dirac cone structure.<sup>7</sup> As graphene has no bandgap, there exists a Dirac point where the electron and hole concentrations are equal, resulting in the smallest current level at this point. In our experimental results, the Dirac point voltage ( $V_{Dirac}$ ) is nearly 0 V, as shown in Figure S10a. However, when the gate bias exceeds the Dirac point voltage, electron conduction is allowed, and when it is below the Dirac point voltage, hole conduction is allowed, with the current increasing in both cases. Figure S11 indicates that  $I_{DS}$  increases as the absolute value of  $V_{GS} - V_{Dirac}$  increases. However, unlike semiconductor FETs, graphene FETs do not exhibit saturation in the output curves, as shown in Figure S11. As mentioned above, graphene does not exhibit semiconducting properties because there is no bandgap. Consequently, depletion does not occur within the channel near the drain region as in semiconductor FETs, indicating that pinch-off does not occur in the graphene FETs.<sup>8</sup>



**Figure S10.** (a) Representative transfer curves and (b) field-effect mobility distribution of graphene FETs with AlN sandwich structure and  $Al_2O_3$  sandwich structure. (c) Normalized field-effect mobility plots as a function of temperature for  $MoS_2$  FETs with different interfacial layers.



Figure S11. Representative output characteristics of graphene FETs with (a)  $Al_2O_3$  sandwich structure and (b) AlN sandwich structure ranging from  $V_{GS} - V_{Dirac} = -2$  V to  $V_{GS} - V_{Dirac} = 2$  V (step of 1 V).

### References

 B. Liu, L.-J. Wu, Y.-Q. Zhao, L.-Z. Wang and M.-Q. Cai, *Phys. Chem. Chem. Phys.*, 2015, 17, 27088-27093.

2. A. P. John, A. Thenapparambil and M. Thalakulam, *Nanotechnol.*, 2020, **31**, 275703.

3. G. Polumati, C. S. R. Kolli, V. Selamneni, M. F. Salazar, A. De Luna Bugallo and P. Sahatiya, *Adv. Mater. Interfaces*, 2023, **10**, 2202108.

4. K. Chen, D. Kiriya, M. Hettick, M. Tosun, T.-J. Ha, S. R. Madhvapathy, S. Desai, A. Sachid and A. Javey, *APL Mater.*, 2014, **2**.

Q. Qian, B. Li, M. Hua, Z. Zhang, F. Lan, Y. Xu, R. Yan and K. J. Chen, *Sci. Rep.*, 2016, 6, 27676.

J. Zheng, H. Zhang, J. Lv, M. Zhang, J. Wan, N. Gerrits, A. Wu, B. Lan, W. Wang and S. Wang, *JACS Au*, 2023, 3, 1328-1336.

- 7. A. K. Geim and K. S. Novoselov, *Nat. Mater.*, 2007, **6**, 183-191.
- D. Reddy, L. F. Register, G. D. Carpenter and S. K. Banerjee, J. Phys. D Appl. Phys., 2011,
  44, 313001.