

## Effect of the HfO<sub>2</sub> passivation on HfS<sub>2</sub> Transistors

T. Kanazawa<sup>1</sup>, T. Amemiya<sup>1,2</sup>, *Member IEEE*, V. Upadhyaya<sup>1</sup>, A. Ishikawa<sup>3,2</sup>,  
K. Tsuruta<sup>3</sup>, T. Tanaka<sup>2,1</sup>, and Y. Miyamoto<sup>1</sup>, *Member, IEEE*

1. Tokyo Institute of Technology, Tokyo, Japan

2. RIKEN, Wako, Japan

3. Okayama University, Okayama, Japan

E mail: kanazawa.t.aa@m.titech.ac.jp

**Abstract**— Hafnium Disulfide (HfS<sub>2</sub>) is one of the transition metal dichalcogenides which is expected to have high electron mobility and finite bandgap. However, the fabrication process for HfS<sub>2</sub> based electron devices has not been established, and it is required to bring out the superior transport properties of HfS<sub>2</sub>. In this report, we have investigated the effects of ALD HfO<sub>2</sub> passivation on the current properties of HfS<sub>2</sub> Transistors. HfO<sub>2</sub> passivation of HfS<sub>2</sub> surface achieved the improvement in drain current and significant reduction of hysteresis. The charge trapping at the outermost surface seems to be the dominant factor for degradation of the current stability.

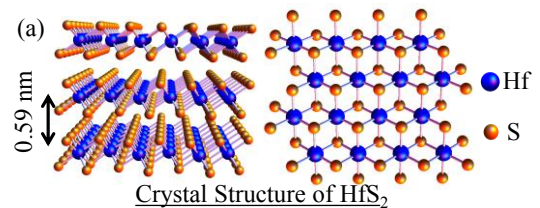
### I. INTRODUCTION

Discovery of the graphene [1] leads the enormous interest in the field of two-dimensional (2D) materials with atomic layer thickness. Graphene shows ultra-high mobility along with other attractive properties and its device applications such as transistors, photodetectors, and gas sensors have been widely studied. However, the absence of bandgap in graphene makes it difficult to suppress the off leakage current of metal-oxide-semiconductor field-effect transistor (MOSFET), which is one of the most important performance parameters for low-power logic applications. Therefore, in recent years, various kind of Transition metal dichalcogenides (TMDs), such as MoS<sub>2</sub> [2], [3] and WSe<sub>2</sub> [4], have been investigated as the post-graphene 2D materials for extremely scaled low-power and high-speed logic applications. These TMDs have both the finite bandgap and extremely thin layer structure (<1 nm), which is attractive for the MOSFETs with the channel length lesser than 10 nm.

Hafnium disulfide (HfS<sub>2</sub>) is one of the semiconducting TMDs, which has the 2D crystal structure with octahedral coordination and single layer thickness of 0.6 nm. HfS<sub>2</sub> is expected to have high acoustic phonon limited electron mobility (~1,800 cm<sup>2</sup>/Vs) [5] and adequate bandgap (1.2 eV~) [6] as shown in Fig. 1. Previously, we reported the device operation of few-layer HfS<sub>2</sub> MOSFETs with robust current saturation and good on/off ratio [7], [8]. Some other groups also reported the electrical properties of HfS<sub>2</sub> FET from theoretical [9] and experimental [10], [11] approaches. However, the maximum drain current of reported HfS<sub>2</sub> FETs were only several hundreds of nA/μm because the fabrication process for HfS<sub>2</sub> MOSFETs has not been established yet. Additionally, in several cases, large hysteresis and high instability of drain current against measurement sequence

were observed due to the charge traps. Moreover, time-dependent degradation of FET current in the atmosphere popped out on continuous evaluation [11], [12]. The atmospheric degradation is one of the critical issues to achieve the high-performance operation of HfS<sub>2</sub> FETs. The degradation seems to be caused by the reaction between HfS<sub>2</sub> surface and moisture, oxygen and other contaminants in the air. To prevent this degradation and instability, the surface of 2D material should be passivated and isolated from the atmosphere to reduce the trap states and absorption of gas atoms, respectively. Previously, the effects of PMMA passivation on HfS<sub>2</sub> FET were observed [12]. Although it indicated some improvement in current performance, the protection using polymer was not beneficial enough to steadily protect the surface from the atmosphere.

In this report, we have investigated the effects of surface passivation by atomic layer deposition (ALD) of HfO<sub>2</sub> dielectric, which is commonly used material as the high-k gate insulator of MOSFETs. The significant reduction in hysteresis was obtained compared to bare devices measured in the atmosphere.



(b) Electrical properties of HfS<sub>2</sub> and typical TMDs

Parameter	Ref.	HfS <sub>2</sub>	MoS <sub>2</sub>	WSe <sub>2</sub>
$\mu_{n,AP}^{\dagger}$ [cm <sup>2</sup> /Vs]	[5]	1,833	340	703
$m^*$ [ $m_0$ ]	[5]	0.24/3.3	0.45	0.33
$E_g$ [eV]	[6]	1.23	1.59	1.32

<sup>†</sup>acoustic phonon limited electron mobility

Fig. 1 (a) crystal structure and (b) fundamental electrical properties of HfS<sub>2</sub>

### II. DEVICE STRUCTURE AND FABRICATION

Figure 2 describes the schematic of the fabricated device structure with optical microscope images of the HfS<sub>2</sub> flake after exfoliation and completed device structure, which is covered by HfO<sub>2</sub>. HfO<sub>2</sub> cap layer caused a change in the color of flakes. Multi-layer HfS<sub>2</sub> has been used as the channel of the MOSFETs. HfO<sub>2</sub> passivation layer was deposited to

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encapsulate the channel and contacts. Gate bias was applied from the degenerately doped Si substrate as the back gate.

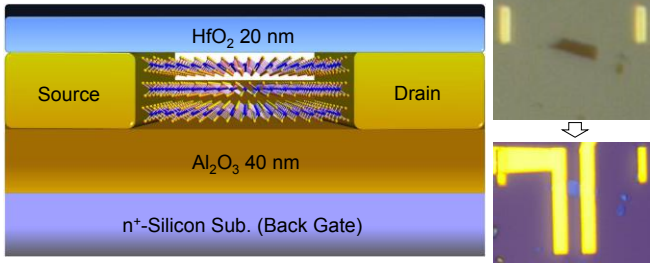


Fig. 2 Schematic device structure and optical images

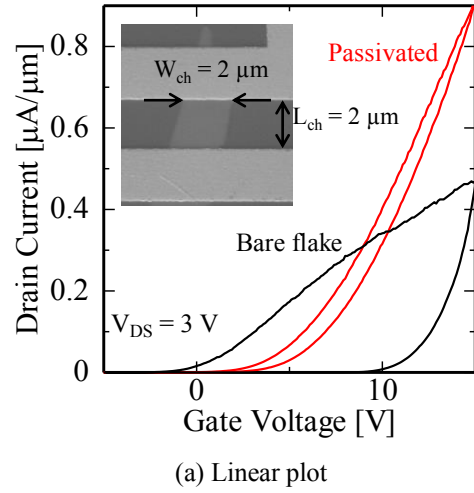
The fabrication process of MOSFETs based on mechanical exfoliation is as follows. First, the back-gate insulator was formed by the ALD of the 40-nm-thick  $\text{Al}_2\text{O}_3$  on  $n^+$ -Si. Secondly,  $\text{HfS}_2$  flakes were transferred to the substrate by the micromechanical exfoliation using polymer adhesive tape with preparing the oxide surface by UV/ozone cleaner. Source/drain (S/D) electrodes and back gate contact were fabricated by the electron beam (EB) lithography and EB evaporation of Ti 20 nm/Au 60 nm and Cr 20 nm/Au 100 nm, respectively. Next, the samples were passivated by  $\text{HfO}_2$ , which was also deposited by ALD at  $150^\circ\text{C}$  using the precursors of Tetrakis(dimethylamino)hafnium (TDMAH) and  $\text{H}_2\text{O}$ . Then, contact holes to S/D electrodes were formed by  $\text{CF}_4$  reactive ion etching of  $\text{HfO}_2$ . Finally, sample annealing was carried out to improve the  $\text{HfS}_2/\text{HfO}_2$  interface and contact properties at  $250^\circ\text{C}$  in vacuum for 10 min. The fabricated devices were measured by the semiconductor parameter analyzer.

### III. RESULTS AND DISCUSSIONS

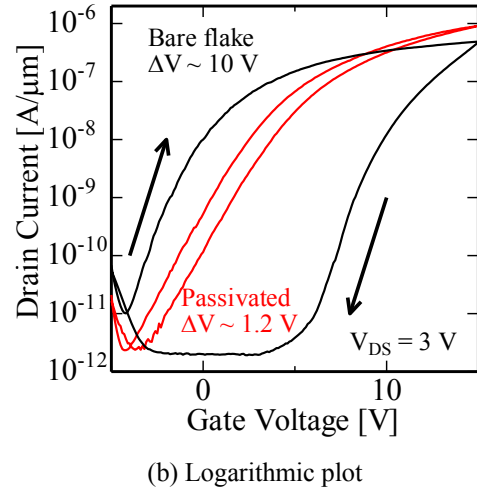
Figure 3 indicates the transfer characteristics of  $\text{HfS}_2$  MOFETs with the similar back gate structure (40-nm-thick  $\text{Al}_2\text{O}_3/\text{Si}$ ) in (a) linear and (b) semi-log plot. The inset SEM image in (a) is the measured sample as the passivated device. The channel length  $L_{\text{ch}}$  and width  $W_{\text{ch}}$  were estimated to be 2  $\mu\text{m}$ . A typical bare  $\text{HfS}_2$  sample, which had been exposed to air during the measurement, showed the significant voltage shift  $\Delta V$  of around 10 V between forward and backward sweep. In contrast,  $\text{HfO}_2$  passivated device fabricated in this report showed suppressed  $\Delta V$  of less than 1.2 V. This improvement in hysteresis by surface passivation suggests that the charge trapping occurred on the outermost surface of  $\text{HfS}_2$  flake. The off-leakage current was same for with and without passivation because it was dominated by the gate leakage. The maximum drain current at  $V_{\text{DS}} = 3$  V and  $V_{\text{GS}} = 15$  V was 0.9  $\mu\text{A}/\mu\text{m}$  for passivated device. Though this value was more than four times higher than previous reports ([8], [10], [11]), the effect of passivation on the drain current is not yet clear due to the process fluctuation. Further investigation and improvement of the S/D contact formation process would achieve the increase of the drain current and clarify the effects of charge trapping on carrier mobility.

Figure 4 shows the output characteristics of the  $\text{HfO}_2$  passivated device. Robust current saturation behaviors were observed. The drain current at  $V_{\text{DS}} = 3$  V and  $V_{\text{GS}} = 15$  V was around 0.8  $\mu\text{A}/\mu\text{m}$ . The difference of current between transfer and output characteristics was around 10%. It was contrary to bare devices, which shows over 80% difference between

transfer and output measurement due to the charge trapping degradation. Moreover, the time-dependent degradation of the drain current in the atmosphere was prevented by the  $\text{HfO}_2$  capping. Therefore,  $\text{HfO}_2$  provides good protection from the oxidation or absorption of any contaminants from the air.



(a) Linear plot



(b) Logarithmic plot

Fig. 3 Comparison of the hysteresis of the transfer curves between bare and  $\text{HfO}_2$  passivated  $\text{HfS}_2$  MOSFETs.

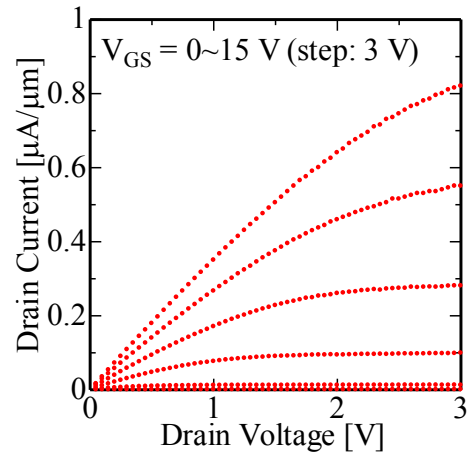


Fig. 4 Output characteristics of  $\text{HfO}_2$  passivated MOSFET.

#### IV. CONCLUSION

In conclusion, we have investigated the effect of surface passivation for HfS<sub>2</sub> MOSFETs using ALD HfO<sub>2</sub>, to improve the stability of the I-V characteristics. The maximum drain current of 0.9 μA/μm was observed at V<sub>DS</sub> = 3 V and V<sub>GS</sub> = 15 V. The hysteresis width ΔV were decreased clearly by the passivation from 10 V to 1.2 V. The protection of the surface by the high-k insulator is an efficient way to reduce the trap charges and improve the stability of properties. The reduction of contact resistance is the next measure to achieve the high current operation.

#### REFERENCES

- [1] K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva, A. A. Firsov, "Electric field effect in atomically thin carbon films." *Science*, vol.306, pp. 666–669, Oct. 2004.
- [2] B. Radisavljevic, A. Radenovic, J. Brivio, V. Giacometti, and A. Kiss, "Single-layer MoS<sub>2</sub> transistors," *Nature Nanotech.*, vol. 6, pp. 217–218, Jan. 2011.
- [3] S. Kim, A. Konar, W.-S. Hwang, J. H. Lee, J. Lee, J. Yang, C. Jung, H. Kim, J.-B. Yoo, J.-Y. Choi, Y. W. Jin, S. Y. Lee, D. Jena, W. Shoi, and K. Kim, "High-mobility and low-power thin-film transistors based on multilayer MoS<sub>2</sub> crystals," *Nature Comm.* Vol. 3, 1011, Aug. 2012.
- [4] W. Liu, J. Kang, D. Sarkar, Y. Khatami, D. Jena, and K. Banerjee, "Role of Metal Contacts in Designing High-Performance Monolayer n-Type WSe<sub>2</sub> Field Effect Transistors," *Nano Lett.*, 2013, vol. 13, pp. 1983–1990. Mar. 2013.
- [5] W. Zhang, Z. Huang, W. Zhang, and Y. Li, "Two-dimensional semiconductors with possible high room temperature mobility," *Nano Research*, vol. 7, pp. 1731–1737, Dec. 2014.
- [6] C. Gong, H. Zhang, W. Wang, L. Colombo, R. M. Wallace, and K. Cho, "Band alignment of two-dimensional transition metal dichalcogenides: Application in tunnel field effect transistors," *Appl. Phys. Lett.*, vol. 103, 053513, Aug. 2013.
- [7] T. Kanazawa, T. Amemiya, A. Ishikawa, K. Tsuruta, T. Tanaka, and Y. Miyamoto "Fabrication of thin-film HfS<sub>2</sub> FET," in *Proc. 73<sup>rd</sup> Device Research Conf.*, Columbus, OH, June 2015, pp. 217–218.
- [8] T. Kanazawa, T. Amemiya, A. Ishikawa, V. Upadhyaya, K. Tsuruta, T. Tanaka, and Y. Miyamoto, "Few-layer HfS<sub>2</sub> transistors," *Scientific Reports*, vol. 6, 22277, Mar. 2016.
- [9] J. Chang, "Modeling of anisotropic two-dimensional materials monolayer HfS<sub>2</sub> and phosphorene metal-oxide semiconductor field effect transistors," *J. Appl. Phys.*, vol. 117, 214502, June 2015.
- [10] K. Xu, Z. Wang, F. Wang, Y. Huang, F. Wang, L. Yin, C. Jiang, and J. He, "Ultrasensitive Phototransistors Based on Fe-Layered HfS<sub>2</sub>," *Advanced Materials*, vol. 27, pp. 7781–7887. Oct. 2015.
- [11] S. H. Chae, Y. Jin, T. S. Kim, D. S. Chung, H. Na, H. Nam, H. Kim, D. J. Perello, H. Y. Jeong, T. H. Ly, and Y. H. Lee, "Oxidation Effect in Octahedral Hafnium Disulfide Thin Film," *ACS Nano*, vol. 10 pp. 1309–1316, Jan. 2016.
- [12] V. Upadhyaya, T. Kanazawa, and Y. Miyamoto, "Vacuum Annealing and Passivation of HfS<sub>2</sub> FET for Mitigation of Atmospheric Degradation," 2016 Asia-Pacific Workshop on Fundamentals and Applications of Advanced Semiconductor Devices (AWAD 2016), A5-7, Hakodate, Japan, July 2016.