## Improvement of HfO<sub>2</sub> on TMDCs using Thermal Expansion Coefficient difference with Substrate

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Recently, two-dimensional Transition Metal Dichalcogenide (TMDCs), such as MoS<sub>2</sub>, have gained attention as next-generation semiconductor materials. However, due to the nature of these 2D materials, which lack dangling bonds that form interlayer bonds, it is challenging to form gate oxide materials like high-k materials. To address this, methods such as plasma or functional group treatment for surface modification of 2D materials and the use of interlayer materials like h-BN have been attempted. However, surface treatment methods can cause damage to the MoS<sub>2</sub> surface, leading to performance degradation, and interlayer materials like h-BN are mostly low-k, requiring very thin EOT formation, which introduces other side effects.

In order to overcome these challenges, methods for directly forming high-k materials via Atomic Layer Deposition (ALD) have been explored. The representative method is the CVD-ALD Mode approach using physical adsorption as a seed due to the low binding energy of 2D materials. While materials like HZO and Al<sub>2</sub>O<sub>3</sub> have been successfully deposited using this method, bulkier materials like HfO<sub>2</sub> tend to form islands and pinholes, resulting in non-uniform growth.

To achieve uniform  $HfO_2$  on  $MoS_2$ , PMMA is used as substrate material which induce strain by thermal expansion coefficient differences. The thermal expansion coefficients of  $MoS_2$  and  $SiO_2$  are generally known to be 7.0 x 10^-6 /K and 0.5 x 10^-6 /K, respectively. The difference in the thermal expansion coefficients between these two materials is 6.5 x  $10^-6$  /K. In contrast, the thermal expansion coefficient of PMMA is around 7.5 x  $10^-5$  /K, indicating a difference of 6.8 x  $10^-5$  /K with  $MoS_2$ , which is more than 10 times higher. Therefore, it is expected that the strain induced by the difference in the thermal expansion coefficient with PMMA will be higher compared to that with a Si substrate. As we expected, uniform  $HfO_2$  is formed on  $MoS_2$  (Fig 1). This method is expected to be utilized in next-generation semiconductor devices structure as it does not damage the channel.



[Figure 1] Overall Process Procedure for Strain: (a) Flake Transfer at 100°C (b) CVD-ALD HfO2 Deposition at 250°C (c) After Cooling at Room Temperature (25°C)

[1] Schilir` oa,\*, S.E. Panascia, and A.M. Mioa, Applied Surface Science 630 (2023)

[2] Stephen McDonnell<sup>\*</sup>, Barry Brennan and Angelica Azcatl, ACS Nano 7/11 (2013)

## **Supplementary Pages (Optional)**



[Figure 2] AFM Image of  $HfO_2$  on  $MoS_2$ : (a)  $MoS_2$  is transferred on  $SiO_2$  (b)  $MoS_2$  is transferred on PMMA.