Effect of Random Nanosized Titanium Nitride Grains on Monolayer MoS_2 Field-Effect Transistors

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ABSTRACT

This work first studies effects of work function fluctuation (WKF) of nanosized titanium nitride (TiN) grains via device simulation on monolayer (ML) molybdenum disulfide (MoS_2) back-gate (BG) and nanosheet (NS) field-effect transistors (FETs). Density functional theory (DFT) calculated data are calibrated with experimental results in order to provide proper accuracy of device simulation. The results indicate that the off-state current and the threshold voltage exhibit the most significant variations. NS FETs are 5% and 2.06% lower variability of these parameters than that of BG FETs.

INTRODUCTION

During the fabrication process of semiconductor devices, work function fluctuation [1-2] is a critical factor associated with process variation effect and intrinsic parameter fluctuation. As researches are focus on two-dimensional (2D) materials for device applications [3-7], challenges of WKF remain difficult to mitigate. Although WKF has been studied in advanced silicon-based devices, study of the effect of WKF on ML MoS_2 devices has not been reported yet.

In this study, to examine the effect of WKF on 2D material-based devices, we first advance the DFT-simulated material parameters for statistical device simulation of ML MoS_2 FETs with nanosized TiN grain of gate.

MODEL AND METHODOLOGY

The 3D device simulation is mainly based on parameters obtained from DFT and calibrated using experimental data. First, DFT calculations are performed to extract key material properties of MoS_2, such as the band gap (E_g), effective mass (m_e^*), and electron affinity (χ_e), which are list in Table 1. The nominal gate metal is TiN with WK = 4.52 eV. To account for fluctuation, the high and low WK values are set to 4.6 and 4.4 eV, respectively, with corresponding probabilities of 0.6 and 0.4, where the grain size is set close to (4 nm)^2, as shown in Fig. 1. For each of above devices, 300 samples are simulated statistically [8] for key DC characteristics, the on-/off-state current (I_{ON} and I_{OFF}), the threshold voltage in linear (V_{th_lin}) and saturation (V_{th_sat}) regions, subthreshold swing (SS), and the drain-induced barrier lowering (DIBL).

RESULTS AND DISCUSSION

First, a BG FET simulation is constructed for calibration with the experimental I_D-V_G curve [7], as shown in Fig. 2. Then, the nominal case of MoS_2 BG FET for the WKF study as well as NS FET are designed, as shown in Figs. 2 and 3. The geometric parameters and DC characteristics are listed in Table 2. Figure 4 shows the fluctuation in results for MoS_2 BG FET and NS FET at V_D = 0.7 V. In the nominal case, V_{th_sat} for both devices is fixed at 140 mV. The standard deviation of the V_{th_sat} for BG FETs is 9.40 mV, which is higher than that of NS FETs (5.84 mV). Furthermore, we estimate the relative standard deviation (RSD), defined as the ratio of the standard deviation to the mean value, for the most significant DC characteristics, as shown in Fig. 5. Figure 6 presents the relationship between the electric potential and the distribution pattern of high/low work function (WKF) metals. In extreme cases where effective WK = 4.52 eV, the BG FET is primarily affected by high WK metal near the source side. In contrast, the NS FET mitigates this effect due to its multi-gate structure.

CONCLUSION

In summary, the analysis of WKF in ML MoS_2 FETs has been studied by using random assigned TiN grains in 3D device simulation. For the given TiN grain size of (4 nm)^2, the NS FET shows enhanced robustness against external variations, as evidenced by its reduced standard variability in DC characteristics compared to the BG FET.

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Table 1. The extracted band gap, electron affinity, and effective mass of ML MoS_2 from DFT simulation.

Material Properties	ML MoS_2
Band gap (E_g)	1.78 eV
Electron affinity (χ_e)	4.26 eV
Effective mass (m_e^*)	4.59 m_0

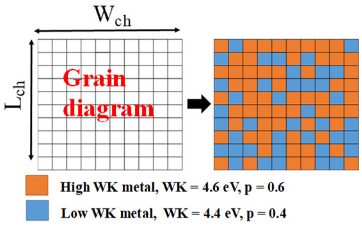

Fig. 1. Illustration of WKF setting.

Table 2. The critical device dimensions and electrical characteristic for MoS_2 BG FET and NS FET without WKF.

Parameter	BG FET	NS FET
L_{ch} (nm)	100	
EOT (nm)	2.448	
W_{ch} (nm)	25	
t_{ch} (nm)	0.42	
EWK (eV)	4.52	
V_{th_lin} (mV)	195	178
V_{th_sat} (mV)	140	140
I_{on} ($\times 10^{-6}$ A)	7.83	3.67
I_{off} ($\times 10^{-11}$ A)	4.66	3.76
SS (mV/dec.)	131	121
DIBL (mV/V)	84.3	60.2

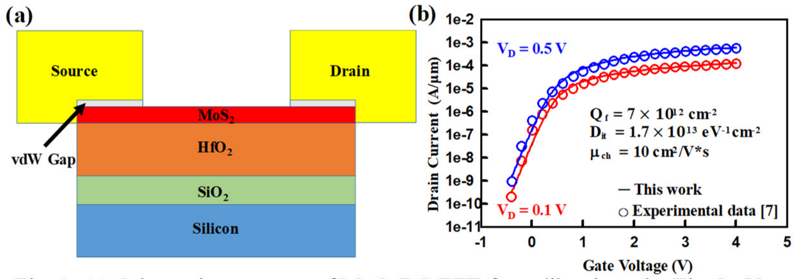

Fig. 2. (a) Schematic structure of MoS_2 BG FET for calibration. (b) The I_D-V_G curves calibrated with fabrication result [7].

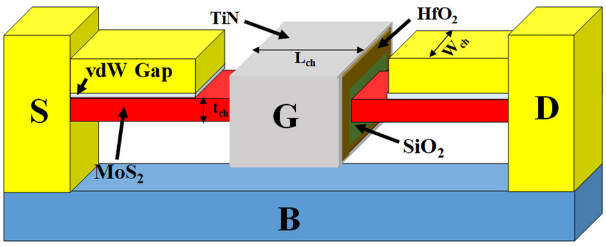

Fig. 3. Schematic of 3D MoS_2 NSFET structure.

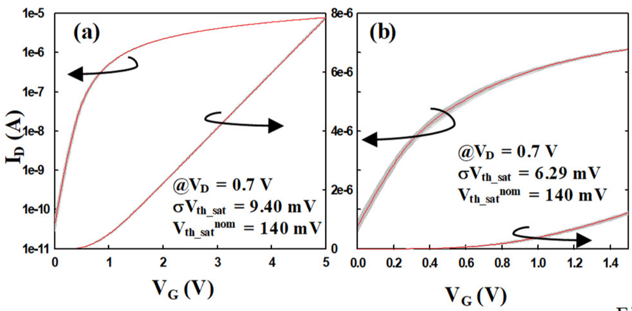

Fig. 4. The fluctuated I_D-V_G results of MoS_2 (a) BG FET (b) NS FET in saturation (V_D = 0.7 V).

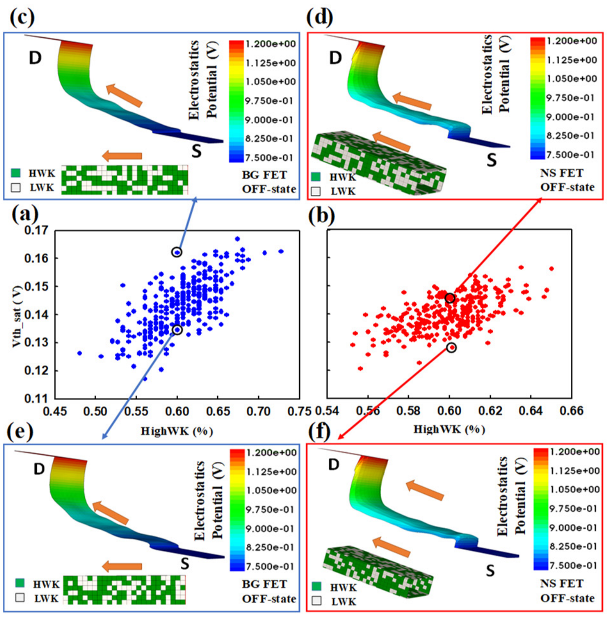

Fig. 6. V_{th} vs the probability of high WK metal for (a) BG FET and (b) NS FET, where (c) and (d) represent high V_{th} case, and (e) and (f) represent low V_{th} case.

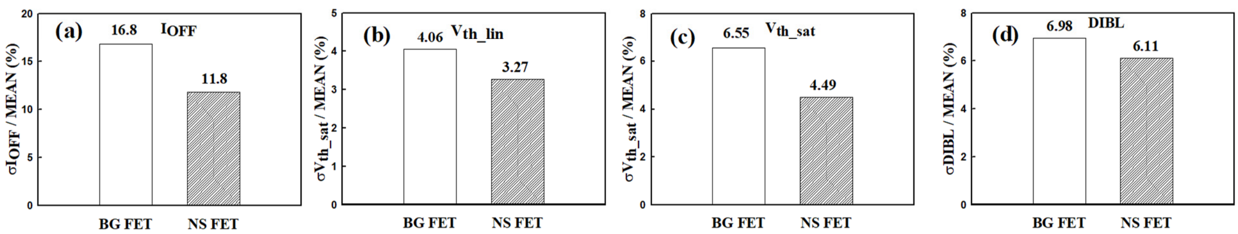

Fig. 5. Normalized fluctuation values comparison between BG FET and NS FET for DC characteristics: (a) OFF-state current, threshold voltage under (b) linear and (c) saturate region, and (d) drain-induce barrier lowering.