High-performance and low-power 2D transition-metal dichalcogenide field-effect transistors

Zhihao Yu¹, Hao Qiu¹, Zhun-Yong Ong², Gang Zhang², Yi Shi¹ and Xinran Wang¹

¹ School of Electronic Science and Engineering, Nanjing University, Nanjing 210023, China Phone: +86-021-89681302 E-mail: xrwang@nju.edu.cn

² Institute of High Performance Computing, 1 Fusionopolis Way, 138632, Singapore

Abstract

Two-dimensional transition-metal dichalcogenides (TMDs) represent a promising class of materials for electronic and photonic devices, benefiting from their high mobility, tunable bandgap and ultrathin body. In this context, we carry out systematic investigations on high performance and low power TMDs field-effect transistors (FETs). We observed large density of atomic defects in monolayer MoS₂ lattice, resulting in hopping transport of MoS₂ transistors, and a facile thiol chemistry can repair the sulfur vacancies and improve the interface quality, leading to significant reduction of impurities and traps. In combination with high- κ dielectrics, we achieve recordhigh room-temperature mobility of ~150 cm²/Vs and 83cm²/Vs for monolayer MoS₂ and WS₂, respectively. We further develop a theoretical model to quantitatively correlate these scattering sources to measured electrical data. For low power application, we realize steep-slope MoS₂ntype negative capacitance FETs (NCFETs) using ferroelectric (FE) HfZrO_x (HZO)/AlO_x as dielectric. The MoS₂ NCFET devices exhibit ultra-low subthreshold swing (SS) of 23 mV/dec, sub-60mV/dec over 6 orders of I_D and nearly hysteresis-free. Our study paves the way for highperformance and low-power applications of TMDs.

1. Introduction

Microelectronic devices continue to develop along the Moore's Law for more than 50 years and are facing challenges such as limitation of physical scaling and high power consumption.¹ The 2D semiconductor, represented by TMDs, with atomic thickness and tunable bandgap show a promising material revolution in electronic and optoelectronics devices. However, the charge transport in monolayer of TMDs is dominated by many extrinsic factors and carrier mobility is still far away from the intrinsic limitation.²

Here, we report the mobility engineering in monolayer MoS_2 and WS_2 by combination of transport theory and experimental methods. Record-high room-temperature mobility of ~150cm²/Vs7 and 83cm²/Vs are achieved for monolayer MoS_2 and WS_2 , respectively. Our combined experimental and theoretical study provides a clear path towards intrinsic charge transport in TMDs for future high-performance device applications.

Furthermore, we report the MoS2 NCFETs using HZO as

a dielectric layer, showing impressive device characteristics, including minimum SS of 23 mV/dec, sub-60 mV/dec operation for over 6 decades, negligible hysteresis. The 2D NCFETs demonstrate new low power application potential for future devices.

2. High Performance TMDs MOSFETs



Figure 1. (a)I_d-V_g characteristics of MoS_2 FET in different ambient (b)On-state current and mobility versus O₂ pressure (c)HR-TEM of monolayer MoS_2 (d)Arrhenius plot of normalized conductivity and the fitting results by hopping model

We report that chemisorption of both oxygen and water from ambient causes degradation of conductance to ~100 times. After annealing *in-situ* at 350 K under high vacuum, the on-state current gradually increased to a stable level of ~5 times higher (Fig. 1a, b). ³To reveal nature of the disorders, we performed HR-TEM characterizations. The HR-TEM shows a large number of sulfur vacancies on MoS₂ (Fig. 1c). Together with DFT calculation, we proposed a transport model in which low-carrier-density transport is dominated by hopping among defect-induced localized states(Fig. 1d).⁴

Next, we employed thiol chemistry to repair the sulfur vacancies(Fig. 2a), resulting in significant reduction of the charged impurities and traps. Record-high mobility greater than 80 cm²/Vs is achieved in back-gated monolayer MoS_2 FET at room temperature(Fig 2b).⁵ Furthermore, we perform a combined experimental and theoretical study of the charge transport in unprecedented phonon-limited mobility of ~150cm²/Vs attained in our samples at room temperature, due to suppression of Coulomb impurity scattering through dielectric and carrier screening.(Fig 2c-d)^{6,7}

Figure 2. (a)Schematic of the reaction between SV and MPS (b) μ -*T* characteristics for the three MoS₂ devices with best theoretical fittings (c)Space distribution of Coulomb potential for a point charge in MoS₂ (d) μ -*T* characteristics for MoS₂ devices on SiO₂ and HfO₂ with best theoretical fittings



To understand the underlying limitations in current MoS_2 FETs, we review the scattering mechnisms and charge traps in MoS_2 from theoretical view, and establish our theoretical model with detailed parameters. Then, we use our model to analyze the available high performance monolayer MoS_2 FET data from literature.(Fig. 3) We shed light on the microscopic origin behind the low mobility in various MoS_2 FET structures.²



Figure 3. Traps and impurities distribution of MoS_2 devices with different processes

3. Low power MoS₂ NCFETs

We report the steep-slope MoS₂ n-type Negative Capacitance Field Effect Transistors (NCFETs) with minimum SS of 23mV/dec using different thickness ferroelectric(FE) HfZrO_x (HZO)/AlO_x as dielectric. The subthreshold slope(SS) and hysteresis of MoS₂ NCFETs show obvious FE thickness dependence. As eclectic results, we find NCFETs on 22nm HZO remain a reduced SS of 23mV/dec without obvious hysteresis.(Fig. 4) Furthermore, we compare the on-current versus on/off ratio of reported and our NCFETs together at defined V_{DD} =0.5V. MoS₂ NCFETs on 22nm and 11nm HZO show large on/off ratio of over 10⁷ with considerable current of over 2µA.⁸ Figure 4. (a)Schematic of MoS₂ NCFET (b)(c)Performance comparison between PCFET and NCFET (d)Thickness dependence of SS and hysteresis for MoS₂ NCFETs



4. Conclusions

We achieved record-high mobility greater than $150 \text{cm}^2/\text{Vs}$ in back-gated monolayer MoS₂ FET at room temperature by defect and interface engineering. Then, we developed a theoretical model to systematically understand the mobility, conductivity, and metal-insulation transition in monolayer MoS₂. Moreover, we demonstrated MoS₂ NCFET with impressive device characteristics using HfZrO_x as gate dielectric for low power applications.

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- Appendix

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