Low-Resistance Contact to Single-Layer MoS₂ by Depositing Ultrathin High-k Dielectric with Remote N₂ Plasma Treatment as Tunneling Layer

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Abstract

Remote N₂ plasma functionalization of single-layer MoS₂ with low damage is explored to deposit ultrathin high-k dielectric on the dangling-bond free single-layer MoS₂. The thin dielectric is used as a tunneling contact layer in source/drain as well as an interfacial layer under the gate to fabricate top-gate MoS₂ MOSFET. The device exhibits mobility as high as 14 cm²/(V·s). The contact resistance significantly drops from 51 kΩ·µm to 11 kΩ·µm, which can be attributed to the alleviated metal-MoS₂ interface reaction and the preserved conductivity of MoS₂ under the source/drain metal contact.

1. Introduction

Molybdenum disulfide (MoS₂), as a semiconductor with atomic-scale thickness and high mobility, has attracted great interests for its promising electronic/optoelectronic applications [1]. However, MoS₂ transistor technology still faces many challenges. Due to the lack of dangling-bonds, it is difficult to deposit high-quality high-k dielectric on MoS₂ as gate dielectric or passivation layer. Moreover, MoS₂ transistor often exhibits large contact resistance. Theoretical calculation suggests that the direct MoS₂-metal contact can introduce gap states through weakening of the Mo-S bonds [2], and XPS results already reveal that interface reactions could happen between MoS₂ and active metals [3]. Not only the interface reaction can cause severe Fermi level pinning, it could also further degrade the conductivity of MoS2 under the contact, resulting in large contact resistance, especially for single-layer MoS₂. In this paper, an ultrathin high-k dielectric layer is deposited on dangling-bond free single-layer MoS₂ using remote N₂ plasma as surface functionalization via Natom adsorption. The thin dielectric is used as a tunneling contact layer to fabricate top-gate MoS₂ MOSFET with reduced contact resistance and high current density.

2. Experiments

Single-layer MoS_2 is prepared on sapphire by CVD. The nearly continuous MoS_2 layer is then transferred to Si substrate capped with 300-nm SiO₂. Remote N₂ plasma shows great advantage as surface functionalization of single-layer MoS_2 [4]. A PEALD system (plasma-enhanced atomic layer deposition, Oxford Instruments OpAL) is used to generate the remote plasma. As shown in Fig. 1, with 10-min remote N₂ plasma treatment as surface functionalization, 5-nm ZrO₂ deposited *in-situ* (200 °C) on single-layer MoS_2 shows greatly improved surface morphology with no pin-holes.



Fig. 1 AFM images of single-layer MoS_2 after ALD 5-nm ZrO_2 (a) without any surface treatment and (b) with 10-min remote N_2 plasma treatment as surface functionalization.



Fig. 2 (a) Raman spectra of fresh single-layer MoS_2 (black), MoS_2 after 10-min remote N_2 plasma treatment (red) and MoS_2 with 3-nm Ti directly deposited on top (blue). (b) Raman spectra of single-layer MoS_2 with thin ZrO₂ deposited on top without/with remote N_2 plasma pretreatment, followed by e-beam evaporation of 3-nm Ti.

The direct metal deposition on MoS2 is often used as contact for MoS₂ MOSFET. However, the weakened Mo-S bonds or even severe interface reactions between metal and MoS₂ could be responsible for the large contact resistance [2], [3]. As shown in in Fig. 2(a), after the deposition of 3-nm Ti on MoS₂, Raman measurement indeed reveals that abundant of defects are generated [5]. Meanwhile, the remote N₂ plasma treatment for 10 min only causes moderate change in the Raman spectra, indicating low-density defects. Thin high-k dielectric deposited on MoS₂ by remote N₂ plasma can be used as a tunneling layer to decouple the MoS₂ surface from the active contact metal. The effectiveness of remote N2 plasma functionalization in promoting uniform dielectric deposition is verified by the Raman spectra in Fig. 2(b). With the remote N₂ treatment, deposition of ZrO₂ as thin as 2 nm can significantly suppress the acoustic-phonon Raman by separating the active metal from MoS₂.

Single-layer MoS_2 MOSFETs with ultrathin high-k dielectric (ZrO₂) deposited by remote N_2 plasma treatment as tunneling contact layer are fabricated. The device structure is



Fig. 3 (a) Schematic of single-layer MoS₂ MOSFET with thin ZrO₂ (red) as tunneling contact layer. (b) Transfer curves for devices with varied tunneling ZrO₂ thickness measured at $V_D = 2 V$. (c) Mobility and (d) contact resistance extracted by Y-function method for different drain voltages.

shown in Fig. 3(a). 5-nm ZrO₂ is adopted as a substrate layer to boost the carrier mobility [1]. The tunneling contact layer thickness is varied from 2 to 4 nm. The top gate dielectric stack features an overall 10-nm ZrO₂ and a 10-nm Al₂O₃ deposited in sequence using thermal ALD. The Al₂O₃ layer is used to better passivate ZrO₂ and stabilize the transistor performance [6]. All the devices have the same channel dimensions of 3 µm in both width and length, with gate overlapping the source/drain by 100 nm. The source/drain contact length is 1 µm. Fig. 3(b) plots the transfer and transconductance curves. At $V_D = 2 V$, the ON current for device with 2-nm ZrO₂ tunneling layer is almost 3 times as large as that without tunneling layer (i.e. 0 nm ZrO₂). Thick tunneling layers (3 nm and 4 nm) result in suppressed ON-current due to large contact resistance from the thick tunneling barrier.

Using the Y-function method [7], the mobility and contact resistance are extracted and shown in Fig. 3(c) and Fig. 3(d). All devices exhibit similar mobility within a range of 8-14 $cm^2/(V \cdot s)$, which are almost independent of the drain voltage, suggesting the effectiveness of the Y-function method. With increased drain bias, the contact resistance drops significantly for device with a tunneling contact. Especially for device with 2-nm ZrO₂ as tunneling contact layer, the contact resistance significantly drops from 51 k Ω ·µm to 11 k Ω ·µm, leading to significantly higher current than the device without tunneling contact, as shown in Fig. 4(a) and Fig. 4(b). Compared with previous work using an evaporated 2-nm MgO as the tunneling contact layer ($R_{on} = 190 \text{ k}\Omega$) [8], our device shows much smaller total resistance ($R_{on} = 30 \text{ k}\Omega$) even with a relatively longer channel. For transistor with thicker tunneling layer, as shown in Fig. 4(c) and Fig. 4(d), larger drain voltage is needed to turn on the tunneling contact and induce stronger tunneling current.



Fig. 4 (a) Output characteristics of single-layer MoS₂ MOSFET without tunneling contact layer. Output curves of MoS₂ MOSFET with (b) 2-nm, (c) 3-nm and (d) 4-nm ZrO₂ as tunneling contact layers. The drain currents are normalized by channel width.

3. Conclusions

Remote N₂ plasma is employed as surface functionalization to deposit ultrathin high-quality high-k dielectric on the dangling-bond free single-layer MoS₂. The dielectric can isolate the MoS₂ from the active metal, as verified by the acoustic-phonon Raman spectra. The deposited dielectric is further used as tunneling contact layer to fabricate top-gate MoS₂ MOSFET. With ultrathin high-k dielectric as tunneling contact layer, the contact resistance significantly drops from 51 k\Omega·µm to 11 kΩ·µm. As a result, the on current increases from 20 µA/µm to 56 µA/µm.

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