A Calibrated Mobility Model for Monolayer Molybdenum Disulfide Device Simulation

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Abstract

This work reports a physical-based mobility model including remote phonon and coulomb scatterings for device simulation of monolayer (ML) molybdenum disulfide (MoS_2) devices. The results adding with electronic structure of ML MoS_2 using density functional theory (DFT) simulation as well as calibrating the contact resistance can properly fit edge contact gate-all-around (GAA) nanosheet (NS) and top contact back gate (BG) FETs well.

Introduction

Recent studies have showed when MoS_2 is deposited on high-κ thin layer oxide, such as HfO_2 and Al_2O_3, it exhibits a higher mobility [1-2]. MoS_2 devices may have superior characteristics and have been studied as a potential candidate for advanced CMOS technologies [3-4]. Computationally, MoS_2 devices are simulated by DFT with nonequilibrium Green's function (NEGF) [5] which provides the most accurate results; however, huge computational resources limit studies of complicated cases. Thus, integrating DFT calculation into device simulation, after validation with results of DFT and NEGF, enables us to explore devices effectively [6].

This study implements a physical-based model by carefully calibrating with Boltzmann transport equation (BTE) for ML MoS_2 device simulation. By adding tunneling gap and contact resistance, we do further calibrate the results with fabricated devices.

The Device Simulation

The results of DFT simulated ML MoS_2 are listed in Table 1. We model the mobility based on remote coulomb scattering (RCS) and remote phonon scattering (RPS) and enhance the accuracy of device simulation by calibrating the results with BTE based on coulomb and phonon scatterings [7, 8] (Fig. 1). It is then applied to device simulation of edge contact GAA NS and top contact BG FETs [3, 7] (Fig. 2). For metal contacts, different simulations are considered for edge and top contact, respectively, devices. In the edge contact, contact resistance is included at the source and drain (S/D), while in the top contact, Wentzel-Kramers-Brillouin (WKB) tunneling with a Schottky contact is used at the interface between the S/D and the varying tunneling gap. The Schottky barrier height between S/D and MoS_2 channel is -0.05 eV. The thickness of tunneling gap (Fig. 3), based on the relaxation of DFT simulation, considers Antimony (Sb) and Bismuth (Bi) contacts.

Results and Discussion

According to the BTE transport, coulomb impurities scattering could be the most significant effect in MoS_2 mobility. If positive charge appears in the channel of MoS_2, due to the 2-D properties of MoS_2, showing screening potential at both sides of the oxide. This causing the coulomb impurity scattering appears. For the coulomb impurity scattering using remote coulomb scattering, we have

$$\mu_{rcs} = \mu_{rcs0}\left(\frac{c}{c_0}\right)^{\gamma_{rcs}} \quad (1)$$

where μ_{rcs} and μ_{rcs0} are the factors for calibration, c is the electron density, and $c_0 = 1.4\times10^{19}$ cm^{-3}. For the phonon scattering, based on conventional phonon scattering μ_{ph} with remote phonon scattering, it is

$$\mu_{rps} = \frac{\mu_{rps0}}{\left(\frac{F_\perp}{10^6\ \mathrm{V/cm}}\right)^{\gamma_{rps}}} \quad (2)$$

$$\mu_{ph\_theory} = {\mu_{ph}}^{-1} + {\mu_{rps}}^{-1} \quad (3)$$

where $F_\perp$ is the transverse field, μ_{rps0} and γ_{rps} are the calibration factor. Matthiessen rule in Eq. (3) adding coulomb and phonon mobility in Fig. 1(b) shows the result that could calibrate with BTE under the values of calibration factors in Table 2.

The mobility and electronic structure from DFT are used for device simulation of edge contact 40 nm gate length GAA NS FET (listed in Table 3). By adding the contact resistance from S/D showing with the calibration on phonon mobility factor matches the I_D-V_G curve (Fig. 4). We then explore the fabricated top contact devices. Due to the ultrathin body of MoS_2, making the top contact of S/D forming an inevitable tunneling gap. Using the First-principle method for relaxation between the metal and MoS_2, Fig. 5 shows the results of top contacts of Sb and Bi. The tunneling gap of two semimetal contact are equal to 3Å and 5Å. By using the calibration of phonon scattering, the calibration of I_D-V_G curve of contact with Sb and Bi are fitting well. The detail results for the calibration of BG FET are listed in Table 4.

Conclusion

We have reported a physical-based mobility model based on remote coulomb and phonon scatterings for ML MoS_2 device simulation. Considering the effects of contact resistance, we have fitted the fabrication results of edge contact GAA NS FET and top contact BGFET by calibrating the phonon scattering factors. Mentioned of the top contact of BGFET, we adding tunneling gap can lead to further simulating the transfer length and contact length.

Table 1. Listed of DFT simulated electronic structures including bandgap, electron affinity, effective mass, dielectric constant, and channel thickness.

Electrical Properties	ML MoS_2	silicon
Band gap (E_g)	1.78 eV	1.12 eV
Electron affinity (χ_e)	4.26 eV	4.08 eV
Effective mass (m_e^*)	4.59 m_0	0.19 m_0
Dielectric constant (ε)	4.8 ε_0	11.7 ε_0
Channel thickness (t_{ch})	0.65 nm	5 nm

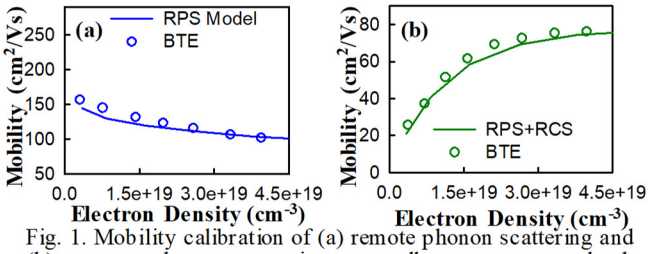

Fig. 1. Mobility calibration of (a) remote phonon scattering and (b) remote phonon scattering as well as remote coulomb scattering, comparing with BTE model [7, 8].

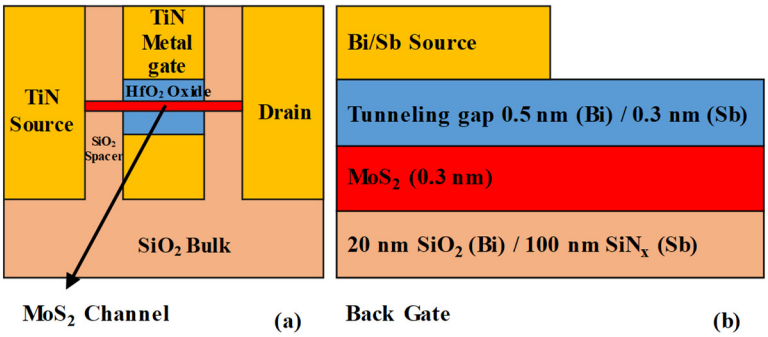

Fig. 2. Schematic plot of the (a) edge contact GAA NS FET and (b) top contact BG FET, where the detail properties of the structure are listed in Table 3.

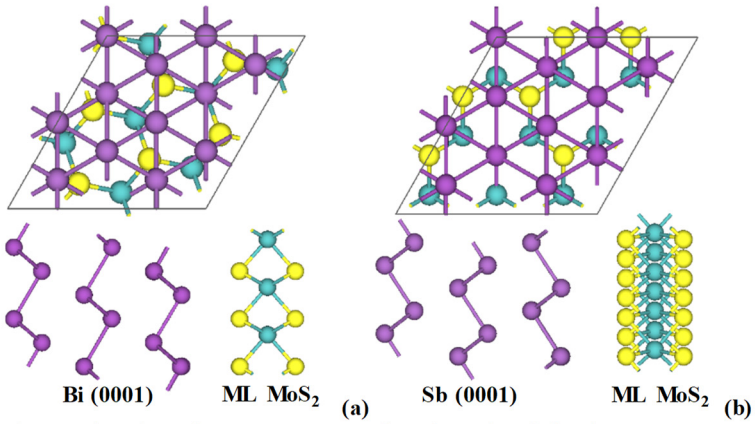

Fig. 3. Relaxation of top contact properties of (a) Bi and (b) Sb.

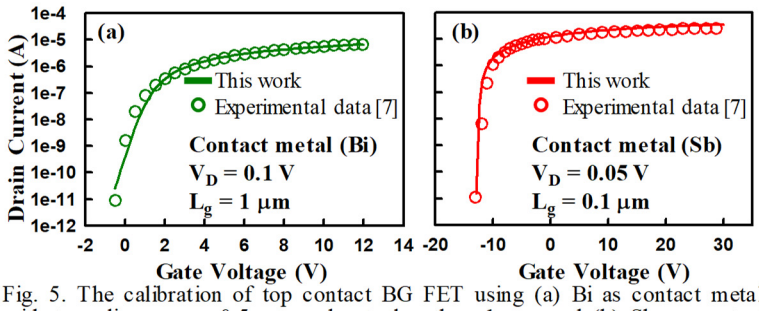

Fig. 5. The calibration of top contact BG FET using (a) Bi as contact metal with tunneling gap = 0.5 nm and gate length = 1 μm and (b) Sb as contact metal with tunneling gap = 0.3 nm and gate length = 0.1 μm.

Table 2. The extracted parameters of the remote coulomb scattering and the remote phonon scattering of the explored mobility of the ML MoS_2, calibrating with BTE model.

Factors	Value
μ_{rcs0}	8
μ_{rps0}	280
g_{rcs}	1.15
g_{rps}	0.5
μ_{ph}	350

Table 3. The detail structure parameters of edge contact GAA NS FET.

Parameter	Value
L_g	40 nm
W	50 nm
t_{ox}	5 nm
EOT	0.9 nm

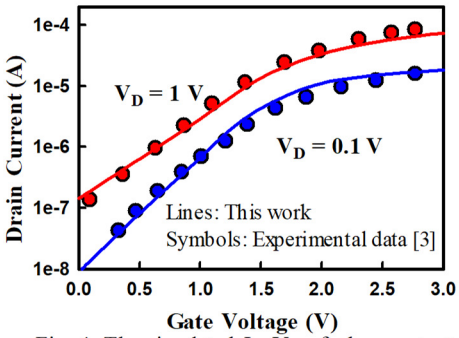

Fig. 4. The simulated I_D-V_G of edge contact GAA NS FET at linear (V_D = 0.1 V) and saturation (V_D = 1 V) regions.

Table 4. List of the calibrated parameters of Bi and Sb BG FETs.

Metal	Bi	Sb
Interface traps (cm^{-2}/eV)	1.2×10^{13}	3×10^{12}
Fixed charge (cm^{-3})	-8×10^{11}	6×10^{12}
SBH (eV)	-0.05	-0.05
Oxide	20-nm SiO_2	100-nm SiN_x

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