

Theoretical Investigation of Molybdenum Disulfide (MoS_2) Field-Effect Transistors for Electronic and Optoelectronic Applications

by

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Author's Declaration

I hereby declare that I am the sole author of this thesis. This is a true copy of the thesis, including any required final revisions, as accepted by my examiners.

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Abstract

After the first demonstration of graphene, 2D materials have attracted tremendous attentions in the electronic devices community. Graphene was regarded as a promising material for electronics due to its extremely high carrier mobility. However, graphene is semi-metallic that doesn't have bandgap in its inherent form, which makes it inappropriate for switching devices in digital logic circuits. On the other hand, there exist another class of new 2D materials, transition metal dichalcogenide (TMDCs). They are atomically thin materials with structure of a transition metal atoms (Mo, W) sandwiched by two chalcogenide atoms (S, Te, Se). Due to its thinness and an appropriate bandgap, many research groups have investigated TMDCs field-effect transistors (FETs) and photonic devices. Among many contenders of TMDCs, molybdenum disulfide (MoS_2) is one of the most viable candidates for future digital applications, showing promising characteristics for electronic and optoelectronic switches, including large on/off current ratio, small sub-threshold swing, and high field-effect mobility.

In this thesis, performance of MoS_2 FETs is predicted and investigated by modeling and simulations so that the results can provide guidelines to experiments for fabrications and optimizations. Transport properties are simulated using the non-equilibrium Green's function (NEGF) formalism, which solves Schrödinger equation under non-equilibrium and open boundary conditions. Simulations of these nano-scale electron devices are performed self-consistently between the electrostatic potential and the charges inside the device. Hamiltonian for describing kinetic and potential energy of electrons in the materials is described in effective-mass or tight-binding method.

Even though many experiments demonstrated promising device characteristics of MoS_2 FETs, the investigation on contact-dependent behaviors of them is still in its infancy. In fact, different types of contacts and their quality can significantly affect the performance of such nanoscale devices. Therefore, in this chapter, using the self-consistent quantum transport simulations, the performance variability of MoS_2 FETs based on different types of contacts is investigated. Varying the Schottky barrier in MoS_2 FETs affects the output characteristics more significantly than the transfer characteristics. If doped contacts are realized, the performance variation due to non-ideal contacts becomes negligible; otherwise, channel doping can effectively suppress the performance variability in metal-contact devices. A scaling study also reveals that, for sub-10-nm channels, doped-contact devices can be more robust in terms of switching, while metal-contact MoS_2 FETs can undergo the smaller penalty in output conductance.

MoS₂ also gives intriguing optoelectronic properties that offer practical feasibility of MoS₂ thin-film transistors (TFTs) for photodetector applications. TFTs using single layer or multilayer MoS₂ are showing higher responsivity than that of graphene TFTs in phototransistors. Recently, responsivity of MoS₂ has been drastically increased after various efforts are made to boost it. While multilayer MoS₂ can be more advantageous than single layer MoS₂ for optoelectronic devices in terms of higher density-of-states and wider spectral response, the responsivity of multilayer MoS₂ phototransistors has remained much lower than that of single layer MoS₂ photodevices mainly due to the indirect bandgap of multilayer MoS₂. Here, an alternative approach is introduced and analyzed to obtain high responsivity in MoS₂ phototransistors. Conducted simulations indicate that the gate underlaps play a key role for the enhancement of photoresponsivity. The comprehensive investigations suggest that high responsivity can be achieved in indirect-bandgap multilayer MoS₂ phototransistors by optimizing optoelectronic design. The results further demonstrate the particular potential of multilayer MoS₂ for optoelectronic applications such as touch screen panels, image sensors, solar cells, and communication devices.

Hamiltonian matrix based on effective mass only describes near the conduction band minima for n-type conduction. In principle, tight-binding (TB) method can provide more precise electronic band description of the material, which is utilized in the later part of this thesis to investigate device characteristics of single layer TMDC FETs, especially for MoS₂. As result of the simulations based on the third-nearest-neighbor (TNN) TB parameters, negative differential resistance (NDR) behavior can be observed, which is defined as a phenomenon that current is decreased with increasing applied bias. The significant effects of the negative output characteristics on the device applications are investigated in detail by varying the transverse modes of the band structure.

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I owe my first and deepest gratitude to my supervisor Professor Youngki Yoon. What he provided me was not only the precious chance to pursue a M.A.Sc degree at the University of Waterloo, but also a door to a wonderful new world of nanoelectronics. I am grateful for his teaching, supervision, advice, and attitude towards research, which have helped me shape my academic career. I also appreciate his great support for my applications for various scholarship competitions. I am very fortunate for being able to work with such a passionate scholar, whose commitment to engineering always influences me significantly.

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Chapter 1

Introduction

1.1 Two-Dimensional (2D) Materials

1.1.1 Graphene

Since the first demonstration of graphene – two-dimensional (2D) sheet of carbon atoms – by Andre Geim and Konstantin Novoselov [1], 2D materials have attracted huge attention from all over the world. Even though the first reports [2], [3] on this material was appeared in 1970s, K. Novoselov *et al.* triggered gigantic interest in this material in 2004 through their pioneering mechanical exfoliation. The graphene lattice is composed of hexagons with a carbon atom at the each corner. The bond length between two atoms is 1.42 Å and lattice constant is 2.46 Å. Today many groups can fabricate this interesting and physically unique material.

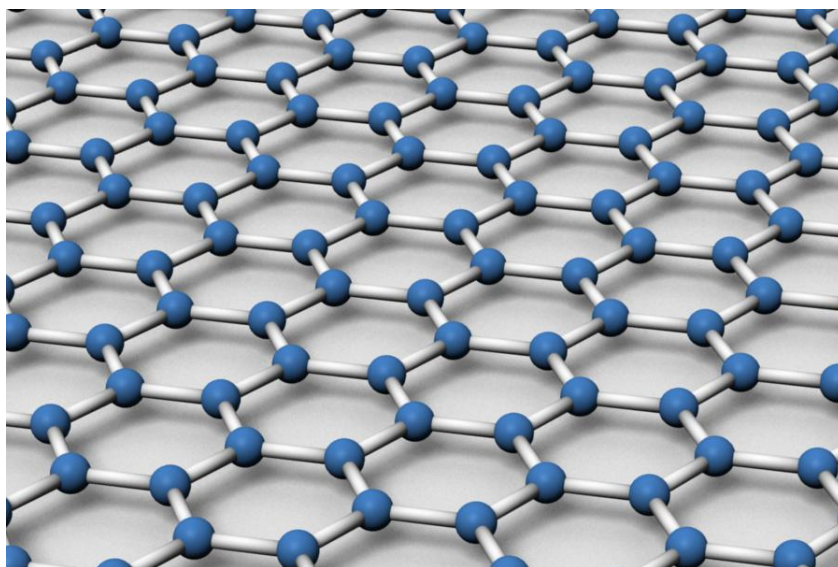


Figure 1.1 Atomistic structure of graphene [4].

At the very early stage, mechanical exfoliation was used to obtain graphene [1]. It can be also grown on metal and transferred to insulating substrates [5], [6]. Another approach is called epitaxial graphene on top of SiC wafers, which is produced by thermal deposition of SiC [7], [8]. Although exfoliation is popular in the laboratory, it is not appropriate for mass production in practice. On the other hand, the other two methods are good for generating large-scale graphene that can be used in

semiconductor process techniques along with lithography and etching towards the fabrication of future graphene-based electronics.

Graphene has cone-shaped valence and conduction band, which meet at the K point in the bandstructure (Fig. 1.2(a) and Fig. 1.2(b)(i)). It can be used for switching applications only with bandgap opening due to its semi-metal nature with zero bandgap. In general, the gap opening can be achieved in three different ways [9]–[28]: (1) confining large-area graphene into one dimension by making graphene nanoribbons (GNRs), (2) applying vertical bias across bilayer graphene, and (3) giving strain to graphene. Zigzag and armchair graphene nanoribbons have bandgaps, where the size of bandgap depends on the width of ribbons and chirality. Even though it is approximately inversely proportional to the width of a nanoribbon, it is hard to achieve a desired bandgap from a graphene nanoribbon since the edges can be easily rough and the width of ribbon can vary along its length. Even two nanoribbons with two different edge geometries show the same bandgap energy due to small edge disorder [14]. Very narrow nanoribbons with well-defined edges are required to open enough bandgap applicable to conventional FETs. Although significant efforts are being made to suppress edge roughness in nanoribbons, perfect edges are still very difficult to achieve. For graphene with a wide bandgap opening, conduction and valence bands close to bandgap become parabolic (rather than cone-shaped). This decrease of curvature around K point degrades performance of the FETs due to the increase of effective mass [29].

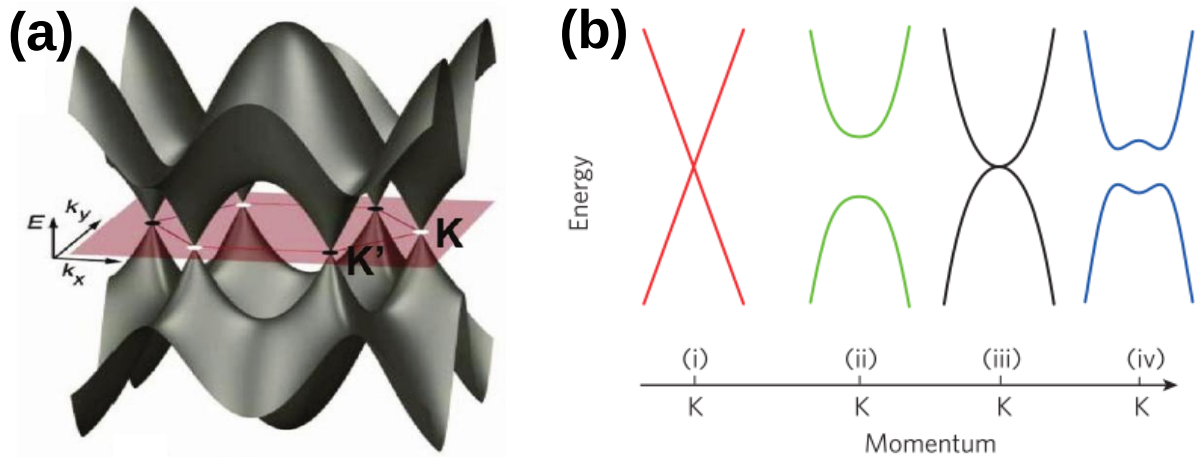


Figure 1.2 (a) 3D bandstructure of graphene [30] (b) Bandstructure around the K point of: (i) large-area graphene, (ii) graphene nanoribbons, (iii) unbiased bilayer graphene, and (iv) bilayer graphene with an perpendicular applied field [31].

Another way to produce a bandgap is to apply a perpendicular electric field to bilayer graphene (see Fig 1.2(b)(iv)). It is reported that the magnitude of the electric field determines the size of bandgap, and an electric field of $1\text{--}3 \times 10^7 \text{ Vcm}^{-1}$ opens a 200–250 meV bandgap [15], [16].

One of the most advantageous properties of graphene is its high electron mobility at room temperature. Due to this property, it has been regarded as a very attractive material for a variety of applications. Typically, exfoliated graphene on SiO₂-covered silicon wafer exhibits mobilities of 10,000–15,000 cm² V⁻¹s⁻¹ and up to 70,000 cm² V⁻¹s⁻¹ is suggested [32], [33]. Moreover, mobilities of 200,000 cm² V⁻¹s⁻¹ have been predicted without charged impurities and ripples [34], and recently suspended graphene exhibited a mobility of 10⁶ cm² V⁻¹s⁻¹ [35].

1.1.2 Transition Metal Dichalcogenides (TMDCs)

A new group of atomistically thin, layered transition metal dichalcogenides (TMDCs) has been demonstrated recently. Many research groups are investigating TMDCs for electronic, chemical, optical, and mechanical applications [36]–[38]. Exceptionally high carrier mobility is shown in graphene, but its low on/off switching ratios and large leakage current limit its use in field-effect transistors (FETs) for switching applications. To improve its characteristics, the bandgap of graphene can be manipulated by restricting the number of lattice as mentioned in section 1.1.1, but it may result in significant mobility degradation. By contrast, several 2D TMDCs possess suitable bandgaps around 1–2 eV [36], [37], providing really good opportunities as FET switching devices.

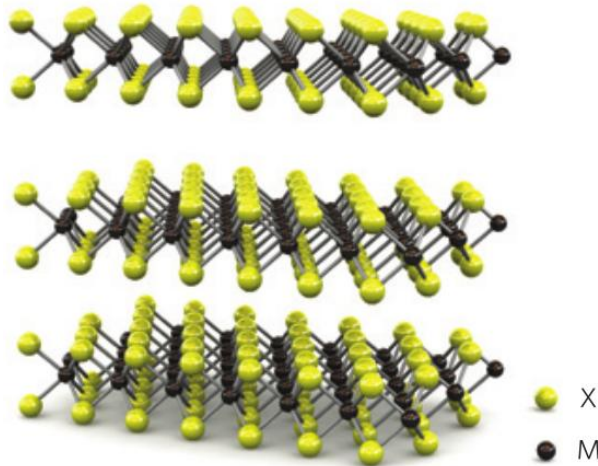


Figure 1.3: TMDCs lattice structure [39].

TMDCs are materials where one layer of M atoms is from group IV (e.g. Ti, Zr, or Hf), V (e.g. V, Nb, or Ta), or VI (Mo or W) is sandwiched between two X atoms (S, Se or Te), as shown in Fig. 1.3. The layers are bound by weak van der Waals force.

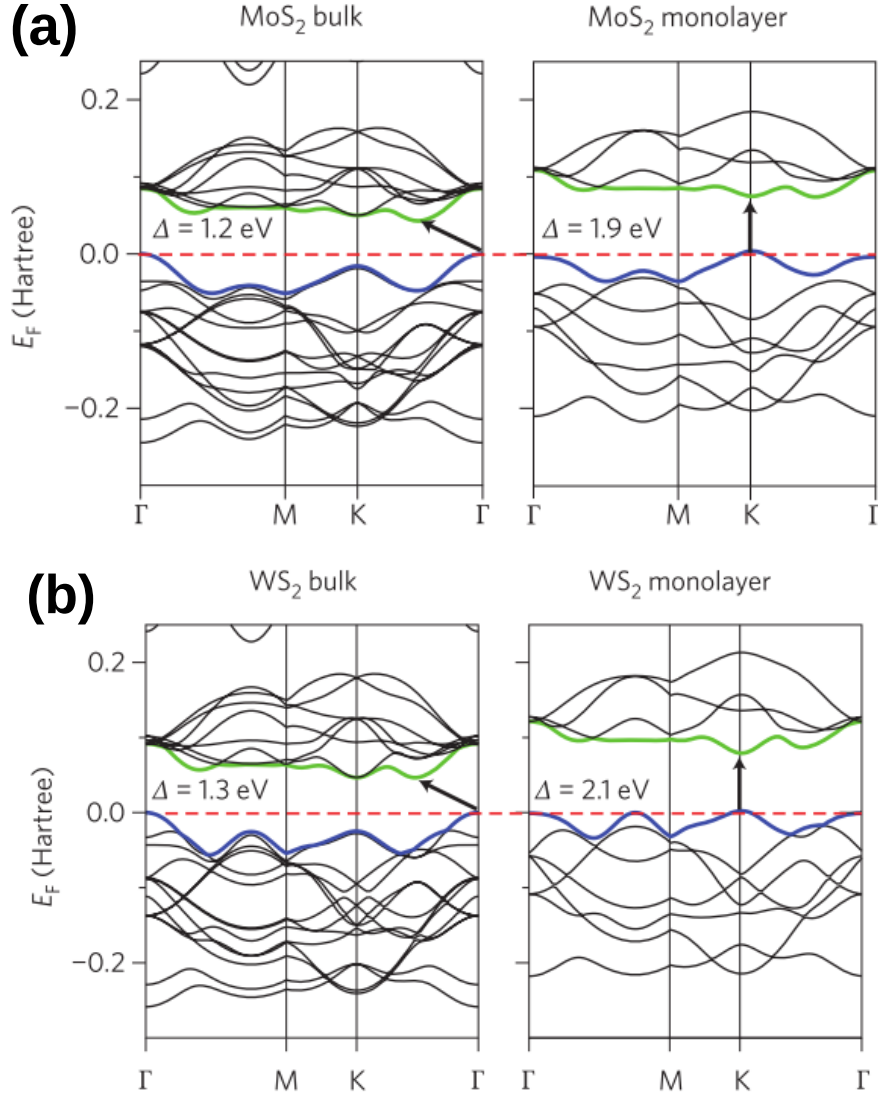


Figure 1.4 Band structures calculated from first-principles density functional theory (DFT) for bulk and monolayer (a) MoS₂ and (b) WS₂. The Fermi level is indicated by the horizontal dashed lines. The arrows indicate the bandgap (direct or indirect). The top of the valence band (blue) and bottom of the conduction band (green) are highlighted [39].

One of the most profitable properties of TMDCs is that their transports depend on the number of layers. For example, whereas bulk MoS₂ has an indirect bandgap of 1.3 eV, monolayer MoS₂ has a

direct bandgap of 1.8 eV. This direct bandgap has positive effects on photoluminescence, which could lead to a breakthrough in optoelectronic applications [40]. Valley polarization is also enabled by the electronic structure of monolayer MoS₂, which bilayer MoS₂ doesn't show [41]–[43].

Many semiconducting TMDCs have similar bandstructures, which is shown by first principles and tight-binding approximation [40][44]–[49]. In general, while some TMDCs such as NbX₂ and TaX₂ are metallic, there are semiconducting TMDCs such as MoX₂ and WX₂ compounds. Figure 1.4 shows the bandstructures of bulk and monolayer MoS₂ and WS₂, plotted from first principles. The bandgap transition at the Γ -point is gradually shifted from indirect for bulk, to direct for monolayer [50]–[55]. The energy gap at the K-point is relatively independent of the layer number compared to other points on the x-axis [56]. Quantum confinement and the resulting hybridization between *d* orbitals on Mo atoms and *p_z* orbitals on S atoms are the reasons for the variation of TMDCs' bandstructure [45], [56], [57].

A transistor is one of the most important semiconductor applications. Metal-oxide-semiconductor field-effect transistors (MOSFETs) have been studied, fabricated and scaled for decades. However, the end of Moore's law is being predicted because successive scaling will approach its limit caused by quantum effects and difficulty in heat dissipation. This circumstance encourages the search for new device designs or materials. Fortunately, 2D semiconductor materials can have immunity to short-channel effects that can limit device performance significantly.

In general, the following characteristics are favorable in field-effect transistors: high carrier mobility for high-speed operation, a high on/off ratio for switching applications, and low off-state conductance for low power applications. To increase the charge density, source, drain or channel materials are doped, which, however, results in scattering and mobility degradation [58]–[60]. For digital logic applications, an on/off ratio of 10⁴–10⁷ is required for switching [31]. Even though graphene is promising for RF applications because of its extremely high carrier mobility and excellent transconductance [31], [61]–[63], it is not suitable for logic applications because the absence of a bandgap results in a large leakage current. Therefore, a new ultra-thin material is required with a reasonable bandgap and large mobility so that a large on/off ratio and a large on current can be achieved.

Among the many possible contenders, molybdenum disulfide (MoS₂) is one of the most viable candidates for future digital applications. It shows promising characteristics for electronic and

optoelectronic switches, including a large on/off current ratio ($I_{ON}/I_{OFF} \approx 10^8$), a small subthreshold swing ($SS = \partial V_G / \partial \log_{10} I_D \approx 70$ mV/decade), and high field-effect mobility ($\mu_{eff} > 100$ cm² V⁻¹s⁻¹).

1.2 State-of-art TMDC Electronic Devices

1.2.1 TMDC Field-Effect Transistors

The earliest TMDC transistor was reported in 2004 where WSe₂ is adopted for the transistor channel, which showed up to 500 cm² V⁻¹s⁻¹ mobility, ambipolar behaviours, and 10⁴ on/off current ratio at a relatively low temperature of 60 K [64]. After that, the first n-type MoS₂ transistor was introduced by Kis, *et al.* [65], as shown schematically in Fig 1.5. The top-gated structure with single layer MoS₂ showed significant on/off current ratio ($\sim 10^8$), large room-temperature mobility (200 cm²V⁻¹s⁻¹), and 74 mV/decade of subthreshold swing (SS). Figure 1.6 shows current-voltage curves for the MoS₂ FET. HfO₂ is used for high-*k* gate dielectric in this device and for boosting the mobility with dielectric engineering [66]. A p-type FET with WSe₂ also used a top-gate geometry with high-*k* dielectric and chemically doped source/drain contacts. This monolayer transistor exhibited hole mobility of 250 cm² V⁻¹ s⁻¹, SS of 60 mV/decade and 10⁶ on/off current ratio [67].

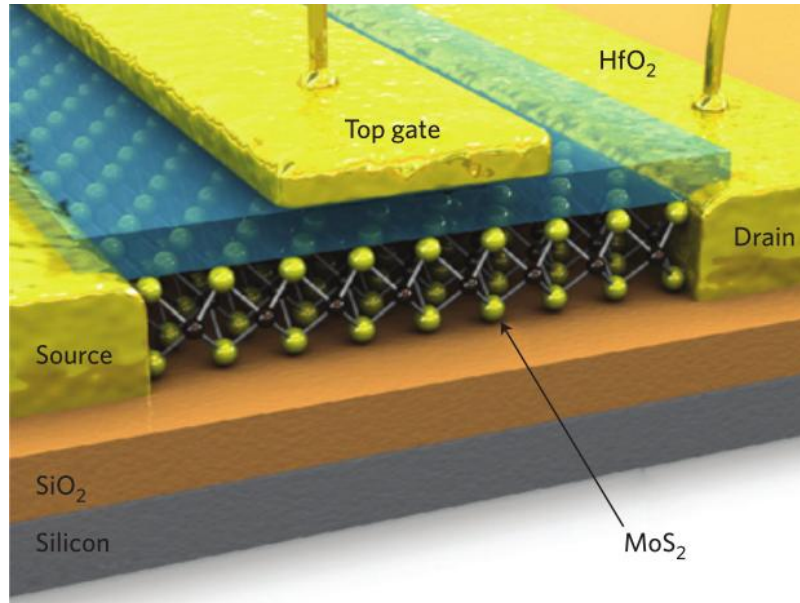


Figure 1.5 Schematic illustration of HfO₂-top-gated monolayer MoS₂ FET device [65].

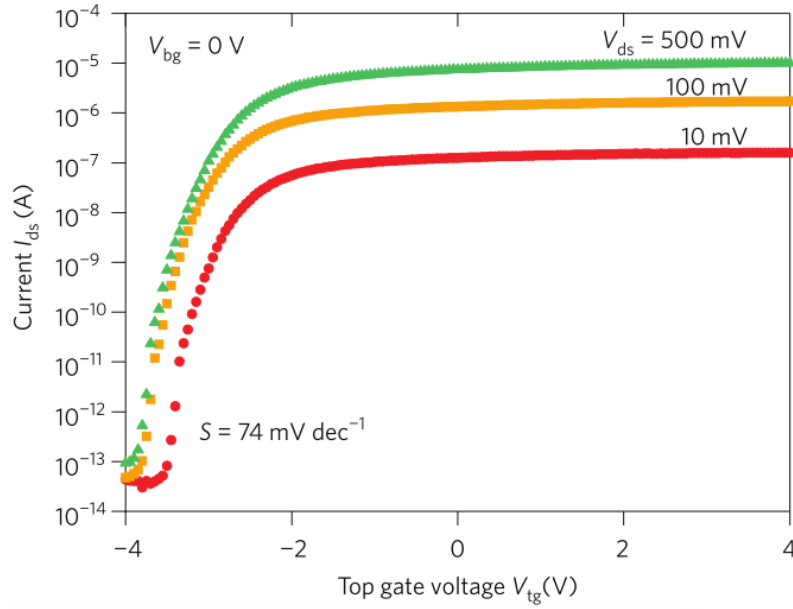


Figure 1.6 Current-gate voltage characteristics of top-gated n-type device in Fig 1.5 [65].

Recently, numerous state-of-art devices using MoS₂ have been investigated. One of them applied atomic-layer-deposited (ALD) high-*k* dielectric integration on MoS₂ crystals and dual-gate n-channel with ALD Al₂O₃ as the gate dielectric, showing high field-effect mobility of electrons [68]. Since the commercial fabrication processes of single-layer MoS₂ with high-*k* dielectric layer are very limited by its compatibility, multilayer MoS₂ FETs are comprehensively investigated and it results in not only high mobilities and near-ideal subthreshold swings as much as single layer MoS₂ FETs, but also robust current saturation over a large voltage window [69].

On the other hand, theoretical simulations have been performed for MoS₂ transistors with short channel effects [46] [60]. Using nonequilibrium Green's function based quantum simulations, top-gated MoS₂ transistors with 15 nm gate length in the ballistic regime were simulated, which predicted 1.6 mA/μm on current, SS of ~60 mV/decade, on/off current ratio 10¹⁰, and immunity to short channel effects (drain-induced barrier lowering of ~10 mV/V). Figure 1.7 indicates simulated transfer characteristics for a monolayer MoS₂ transistor at different drain voltages. It was shown that this simulated MoS₂ transistor is not the best device for high-performance FETs, but it is attractive for low-power applications due to its appropriate bandgap and a large degree of electrostatic control. However, short channel effects at 5 nm channel length double-gated single layer MoS₂ FETs are observed in [70] due to direct source-to-drain tunneling of electrons, which leads to high subthreshold swing.

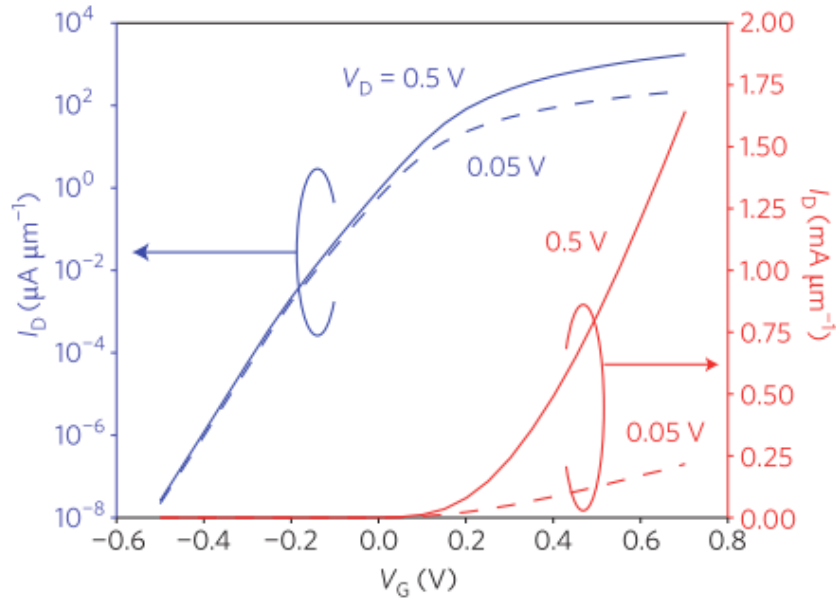


Figure 1.7 Transfer characteristics for a monolayer MoS₂ FET device on linear (right axis) and logarithmic (left axis) scales, simulated by NEGF self-consistent method. The drain voltages (V_D) are 0.05 and 0.5 V [60].

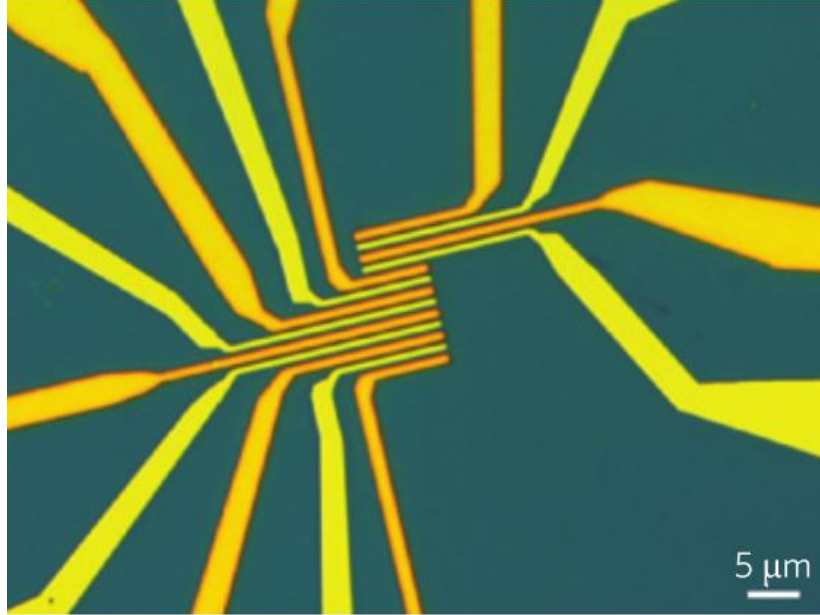


Figure 1.8 Integrated circuit based on single-layer MoS₂ [39].

The first integrated circuits based on MoS₂ have exhibited by Radisavljevic and his coworkers [71]. Lithographically patterning multiple sets of electrode enables fabricating up to six independently

switchable transistors on the same piece of monolayer MoS_2 (see Fig 1.8). Higher than 1 voltage gain at room temperature was measured for the integrated circuit composed of two transistors fabricated on a single flake of MoS_2 , which was operated as logical inverters. A logical NOR gate was also reported, which is one of the most common gates that can be performed by single-layer MoS_2 transistors. Following the first MoS_2 integrated circuit, integrated multistage circuits assembled on bilayer MoS_2 were introduced, including an inverter, a NAND gate, a static random-access memory, and a five-stage ring oscillator [72].

1.2.2 TMDC Phototransistors

Currently, flexible and transparent optoelectronics are expected to become highly significant in solar cells, wearable devices, and transparent displays. In that sense, TMDCs are very promising light-absorbing materials for photovoltaics and photodetectors due to their relatively high Earth abundance and direct bandgap which cause large photoresponsivity. So far, TMDCs are applied to various photovoltaics and photodetectors. Techniques of reactive sputtering and solid-state reactions produce photosensitive textured WS_2 and MoS_2 films [73], and phototransistors made of monolayer MoS_2 have been regarded as a candidate for next generation photodetectors [74]. Good switching behavior of photocurrent generation and annihilation, responding within 50 ms, controllable by the incident light, is shown in the new phototransistor based on single-layer MoS_2 nanosheet produced by the mechanical exfoliation method. Photodetecting different wavelengths is possible by using MoS_2 layers of different thickness. Lee, *et al.*, [75] fabricated multi-layered MoS_2 phototransistors using a transparent gate electrode. They reported that, while triple channel layers with a bandgap of 1.35 eV produce high photodetection capabilities for red light, green light detection is sensed effectively with single and bilayer phototransistors with bandgaps of 1.8 eV and 1.65 eV, respectively. In addition, significant efforts to increase photocurrent through MoS_2 have also been made by plasmonic Au nanoparticles [76].

1.3 Overview of NEGF Transport Simulations

To predict and investigate device characteristics of MoS_2 FETs, transport properties are simulated using the non-equilibrium Green's function (NEGF) formalism [77]–[83][84], which solves Schrödinger's equation under non-equilibrium conditions and open boundary conditions through contacts. A variety of devices from conventional Si MOSFETs [85], MOSFETs of new channel

materials [86], to carbon nano-tube FETs, and molecular transistors have been investigated by the NEGF method [87]. In this section, the basis of the NEGF formalism will be described briefly.

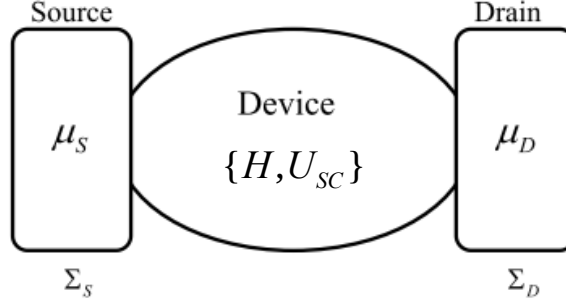


Figure 1.9 Schematic structure of a device where the channel is connected to the source/drain contacts [78].

NEGF formalism represents the device by Hamiltonian, H , and this is contacted to two terminal conductors, source (S) and drain (D) (see Fig. 1.9). In this thesis, the Hamiltonian is based on one-band effective mass or the third-nearest neighbor approximation. Applied bias between the two contacts determines the difference of the Fermi levels (μ_S and μ_D) and how electrons are thermally distributed in each contact through the Fermi function, $f_{S/D}$. Self-energy matrices, Σ_S and Σ_D describe coupling between the active device and the S/D contacts. With knowing H , Σ_S , Σ_D , μ_S and μ_D , we can calculate the retarded Green's function [84] at a given energy as

$$G = [EI - H - \Sigma_S - \Sigma_D]^{-1} \quad (1.1)$$

EI is matrix of electron energy in channel material and also Eigen values of H . In the ballistic regime, the local density-of-states (LDOS) is given by spectral function $[A] = i[G - G^+] = [A_S] + [A_D]$, where $A_{S/D} = G\Gamma_{S/D}G^+$ and $\Gamma_{S/D} = i[\Sigma_{S/D} - \Sigma_{S/D}^+]$ is the energy level broadening due to the source/drain contact. The density matrix [84] is described as

$$[G^n] = [G\Gamma_S G^+]f_S + [G\Gamma_D G^+]f_D \quad (1.2)$$

This is called correlation function. If $f_S = f_D = 1$, then all states are filled with electrons thereby $[G^n]$ becomes local density of states (LDOS). Subsequently, current at source or drain terminal per spin [84] is calculated as

$$I_{S/D} = (e/h) \int_{-\infty}^{+\infty} dE \tilde{I}_{S/D}(E) \quad (1.3)$$

where $\tilde{I}_{S/D} = \text{Trace}[\Gamma_{S/D}A]f_{S/D} - \text{Trace}[\Gamma_{S/D}G^n]$, e and h are free electron charge and Planck's constant, respectively.

1.4 Solving the Poisson Equation

In this section, solving the Poisson equation will be covered by using a double-gate MOSFET as an example based on the finite difference method. Figure 1.10 is the model device structure used in this section.

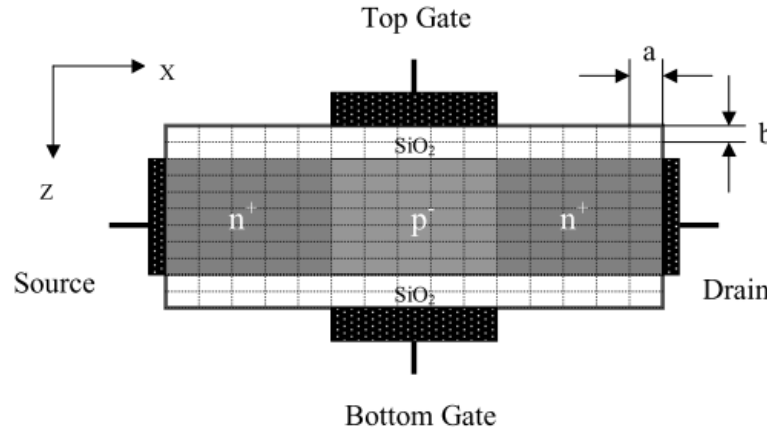


Figure 1.10 Geometry of a thin body double-gate FET. Simulation calculates only region enclosed by the solid line. a and b are spatial constants along the X and Z directions, respectively [83].

Gauss's law enables the Poisson equation to be numeric solution [83]

$$\oint \epsilon \vec{E}(x, z) \cdot d\vec{S} = \int_{\Omega} e[p - n + N_D - N_A] d\Omega \quad (1.4)$$

where ϵ is the dielectric constant which is a function of position, $\vec{E}$ is the electric field, p is the hole concentration, n is the electron concentration, N_D and N_A are donor and acceptor concentrations, respectively, e is a single electron charge. The solution domain of the Poisson equation is composed of $N_x \times N_z$ lattice nodes, where N_x and N_z are the number of nodes in the X and Z directions, respectively. The $N_x \times N_z$ equations are required to get the same number of unknowns. Eq. (1.4) is used to get equations for all internal nodes, while boundary nodes equations are obtained by applying

boundary conditions. For illustrating one node $[m, n]$ (row m and column n) in internal nodes, the finite difference method (FDM) is used for the spatial derivatives. By substituting $\vec{E} = -\nabla V$, the linearized finite difference form [83] from Eq. (1.4) is

$$\frac{a}{b}V_{m-1,n} + \frac{b}{a}V_{m,n-1} - 2\left(\frac{a}{b} + \frac{b}{a}\right)V_{m,n} + \frac{b}{a}V_{m,n+1} + \frac{a}{b}V_{m+1,n} = -\frac{ab}{\varepsilon}e(N_D - N_A - n)_{m,n} \quad (1.5)$$

where a and b are mesh spacings in the X and Z directions, respectively. $\varepsilon = \varepsilon_{ox}/\varepsilon_{ch}$ when node $[m, n]$ is oxide/channel regions. If the node is located at the channel/oxide interface, Eq (1.5) becomes

$$\begin{aligned} \frac{a}{b}V_{m-1,n} + \frac{b}{2a}\left(1 + \frac{\varepsilon_{Bot}}{\varepsilon_{Top}}\right)V_{m,n-1} - \left(\frac{a}{b} + \frac{b}{a}\right)\left(1 + \frac{\varepsilon_{Bot}}{\varepsilon_{Top}}\right)V_{m,n} + \frac{b}{2a}\left(1 + \frac{\varepsilon_{Bot}}{\varepsilon_{Top}}\right)V_{m,n+1} \\ + \frac{a}{b}\frac{\varepsilon_{Bot}}{\varepsilon_{Top}}V_{m+1,n} = -\frac{ab}{\varepsilon_{Top}}e(N_D - N_A - n)_{m,n} \end{aligned} \quad (1.6)$$

where ε_{Top} and ε_{Bot} indicates dielectric constants for the materials above the interface and below the interface [83]. This expression indicates that only charge at $[m, n]$ node and the voltage at the four nearest neighbors determine the voltage of $V_{m,n}$. Graphical depiction of these nodes, which is called computational molecule, is shown in Fig 1.11. Since this is composed of 5 points, this tensile is usually named as the five pointed star.

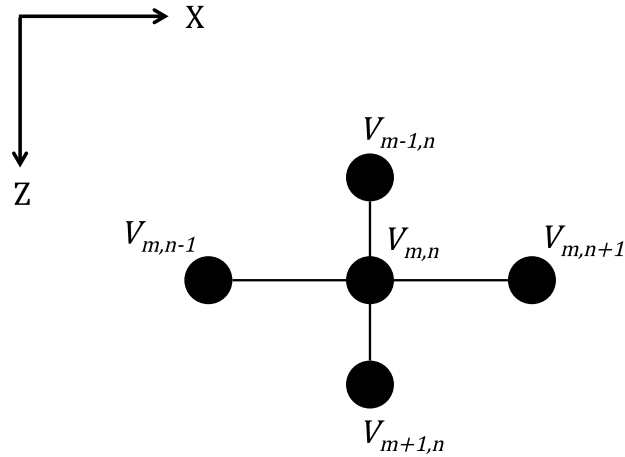


Figure 1.11 Computational molecule for the five pointed star [88].

Next, let's consider equations for all boundary nodes. Confining simulation domain is required since a computer can only process a finite number of grid points. Two most common forms of

boundary condition are the Dirichlet and the Neumann boundary conditions. The former can be written as

$$V(r) = f(r) \quad (r \in \Omega_D), \quad (1.7)$$

where the Ω_D is the set of all nodes which satisfies the Dirichlet condition [88]. This condition is a forced solution to the potential function f at specific points. At the gate contacts in our example, substituting Ω_D with a set of nodes at the interface between gate electrode oxide interfaces, the numerical equation can be easily written as,

$$V_{m,n} = V_G \quad (1.8)$$

where V_G is determined from the gate bias voltage.

On the other hand, if derivative of the potential function is known, the Neumann boundary condition can be used, which is defined as

$$\frac{\partial V(r)}{\partial n} = f'(n) \quad (r \in \Omega_N), \quad (1.9)$$

where n is the surface unit normal vector, and f' is the set of known derivatives [88]. Left-hand side indicates derivative with respect to the unit normal vector at the boundary, called normal derivative. This boundary condition enables contact potentials to be the right values that make charge neutrality be satisfied in the contact regions. If the known derivatives, f' is fixed to 0.0 V/m in our case [83],

$$\begin{aligned} V_{m,n} - V_{m\pm 1,n} &= 0 \text{ for the top and bottom edges,} \\ V_{m,n} - V_{m,n\pm 1} &= 0 \text{ for the left and right edges,} \\ 2V_{m,n} - (V_{m+1,n} + V_{m,n\pm 1}) &= 0 \text{ for the two corner nodes along the top edge, and} \\ 2V_{m,n} - (V_{m-1,n} + V_{m,n\pm 1}) &= 0 \text{ for the two corner nodes along the bottom edge.} \end{aligned} \quad (1.10)$$

At the boundaries except gate and source/drain contacts, we assume the same zero electric field condition.

Now, the solution over all voltage node $V_{m,n}$ can be represented as a simple matrix-vector equation since the node is just linearly dependent on its four nearest neighbors as shown Eq. (1.5). If vector x containing all of the voltage samples within the domain is described as [88]:

$$x = [V_{1,1} \quad V_{1,2} \quad V_{1,3} \quad \dots \quad V_{m,n-1} \quad V_{m,n} \quad V_{m,n+1} \quad \dots \quad V_{N_Z,N_X}]^T \quad (1.11)$$

we can write entire problem as a matrix-vector equation form:

$$Ax = b \quad (1.12)$$

where b is a vector containing all the information about any charge densities and boundary conditions. Solution vector x can be finally calculated just by inverting matrix A .

$$x = A^{-1}b \quad (1.13)$$

Gaussian elimination may be used to obtain reduced memory and shorter time to invert matrix A .

1.5 Self-Consistent Simulation Scheme

In this thesis, simulations of nano-scale electron devices are performed using a self-consistent simulation scheme between the electrostatic potential and the charges inside the device. Let's consider a device connected with terminals. Some lines of electric field are injected into or ejected out of the device (*e.g.*, the gate electrode). Also, contacts connected to the device enable some charge to flow into or out of the device. (*e.g.*, the source/drain contacts). A self-consistent potential $U_{sc}(\vec{r})$ is produced by both factors (see Fig. 1.12). The reason why it is called 'self-consistent' is that the changes in $\rho(\vec{r})$ adjust potential $U_{sc}(\vec{r})$ inside the device, which in turn alters charge density $\rho(\vec{r})$ until both the potential and charge density reach consistent values. For this iterative simulation, two major equations are needed: the Poisson equation and the transport equation. Input and output of the Poisson equation are charge density $\rho(\vec{r})$ and the self-consistent potential $U_{sc}(\vec{r})$, respectively (see Fig. 1.12). As explained in Section 1.4, it is solved by FDM method. To obtain charge density $\rho(\vec{r})$ (or electron density $n(\vec{r})$) in this equation, a full quantum mechanical transport model such as NEGF formalism should be used as introduced earlier in the section 1.3. For fast convergence between the transport and the electrostatics, the Poisson's equation is solved non-linearly with the quasi-Fermi potential energy [17]. To solve this non-linear equation, a numerical Newton-Raphson method is used.

The self-consistent procedure for a quantum mechanical simulation of TMDCs consist of following steps [78]:

1. Given a particular FET structure, we first set Finite Difference Method (FDM) method to discretize all the operators
2. We input initial guess value of $U_{sc}(\vec{r})$ to initiate self-consistent loop (*e.g.*, a potential $U_{sc}(\vec{r})$ of flat band condition or final potential of the any previous simulations, which has closest solution to the self-consistent potential of the current simulation.)

3. For a given $U_{sc}(\vec{r})$, we can write down a suitable Hamiltonian, H , for the device and compute contact self-source and drain energy matrices, Σ_S , Σ_D , respectively.
4. The retarded Green's function is calculated with all above information to produce electron density matrix.
5. With electron density computed in previous step, a Poisson equation is solved for the self-consistent potential, $U_{sc}(\vec{r})$.
6. Step 3–5 are iterated until difference between the newly computed potential and the previous potential is less than specified error.
7. With the final self-consistent potential and the corresponding electron density matrix, the transport current of the device is calculated.

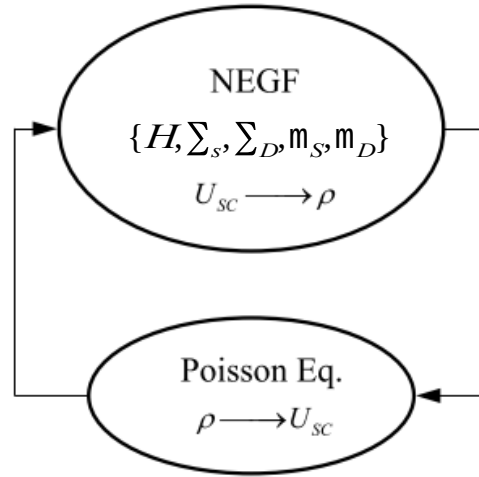


Figure 1.12 The self-consistent diagram iterated by the NEGF formalism and the Poisson equation [78].

1.6 Hamiltonian Matrix

The Hamiltonian H is composed of two parts [84]:

$$H = H_0 + U \quad (1.14)$$

where H_0 is only the isolated materials obtained from information of their bandstructures and U indicates the potential caused by bias voltages. In this section, how to choose the Hamiltonian matrix $[H_0]$ will be illustrated to describe the electronic bands of semiconductor channel in transistors.

1.6.1 Effective Mass Hamiltonian

In chapter 2, the effective mass approximation is adopted to discretize the operators, H . Due to complexity of bandstructure of MoS₂ in conduction and valence band, it is not easy to describe exact H of the material. Effective mass can be adoptable because its description around the low energy level (close to conduction band minima) can be described with a parabola. This simple relation can describe the conduction band minimum as [84]

$$h(\vec{k}) = E_c + \frac{\hbar^2 k^2}{2m_c}, \quad (1.15)$$

where E_c and m_c are conduction band and effective mass of the electron, respectively. A differential equation which has same energy eigenvalues as Eq. (1.15) is easily written down like this [84].

$$\left[E_c - \frac{\hbar^2}{2m_c} \nabla^2 \right] f(\vec{r}) = E f(\vec{r}) \quad (1.16)$$

$f(\vec{r}) = \exp(i\vec{k} \cdot \vec{r})$ with any $\vec{k}$ are eigenfunctions of this differential equation. The corresponding eigenvalues of the eigenfunctions are $E(\vec{k}) = E_c + (\hbar^2 k^2 / 2m_c)$. By using finite difference method (FDM), Eq. (1.16) is converted into a Hamiltonian matrix (*e.g.*, a tridiagonal matrix including $E_c + 2t_0$ on the diagonal and $-t_0$ on the upper and lower diagonals, where $t_0 \equiv \hbar^2 / 2ma^2$ with lattice spacing a) and H_0 can be written as:

$$H_0 = \begin{matrix} & \begin{matrix} 1 & 2 & \dots & N-1 & N \end{matrix} \\ \begin{matrix} 1 \\ 2 \\ \vdots \\ N-1 \\ N \end{matrix} & \begin{bmatrix} 2t_0 & -t_0 & & 0 & 0 \\ -t_0 & 2t_0 & & 0 & 0 \\ & & \ddots & & \\ 0 & 0 & & 2t_0 & -t_0 \\ 0 & 0 & & -t_0 & 2t_0 \end{bmatrix} \end{matrix} \quad (1.17)$$

where N is number of lattice.

1.6.2 Tight-Binding Hamiltonian

The Tight-binding (TB) model is defined as a calculation method for electronic E-K band structure, using an approximate set of wave functions by superposing wave functions for isolated atoms. By using this approach, $[H_0]$ can be constructed. For example, Fig. 1.13 depicts a particular unit cell n connected to other unit cells m surrounding it. Those are called neighbor unit cells. Matrix $[H_{nm}]$ of

size $(b \times b)$ describes connection between the two unit cells, b being the number of basis functions per unit cell. The overall matrix equation in the form can be written as [84]

$$\sum_m [H_{nm}] \{\phi_m\} = E \{\phi_n\} \quad (1.18)$$

where $\{\phi_m\}$ is a $(b \times 1)$ column vector which describes the wavefunction in unit cell m . If solution of this equation is $\{\phi_m\} = \{\phi_0\} e^{i\vec{k} \cdot \vec{d}_m}$ and substitute it into Eq. (1.18) considering periodicity of the lattice, the equation becomes [84]

$$E \{\phi_0\} = [h(\vec{k})] \{\phi_0\} \quad (1.19)$$

with

$$[h(\vec{k})] = \sum_m [H_{nm}] e^{i\vec{k} \cdot (\vec{d}_m - \vec{d}_n)} \quad (1.20)$$

The outcome of this equation is obtained by considering all couplings to its neighboring unit cells (including itself). The size of $[h(\vec{k})]$ is same as that of H_{mn} , $b \times b$. This can be used for plotting the bandstructure. By using a numerical package such as MATLAB, the eigenvalues and eigenfunctions of the $(b \times b)$ matrix $[h(\vec{k})]$ can be easily obtained. And then those eigenvalues become energy levels in bandstructure for each value of $\vec{k}$ at which b branches are located. In contrast, a collection of matrices $[H_{nm}]$ from the Eq. 1.20 can make up the matrix $[H_0]$ representing a periodic solid, which is of size $(Nb \times Nb)$, N being the total number of unit cells. The TB model enables us to calculate H_0 , offering relatively accurate description of bandstructure and lower computational load than the first-principle method. This calculated H_0 is employed to run self-consistent simulation in NEGF formalism as mentioned earlier in section 1.3

In the chapter 4, we chose a minimal symmetry-based three-band TB model using only the d_{z^2} , d_{xy} , and $d_{x^2-y^2}$ orbitals [89]. The energy bands in the entire the first BZ can be well described by including third-nearest-neighbor (TNN) Mo-Mo parameters. Fitting first-principles (FP) energy bands gives the following parameters ($\epsilon_1 = 0.683$, $\epsilon_0 = 1.707$, $t_0 = -0.146$, $t_1 = -0.114$, $t_2 = 0.506$, $t_{11} = 0.085$, $t_{12} = 0.162$, $t_{22} = 0.073$, $r_0 = 0.060$, $r_1 = -0.236$, $r_2 = 0.067$, $r_{11} = 0.016$, $r_{12} = 0.087$, $u_0 = -0.038$, $u_1 = 0.046$, $u_2 = 0.001$, $u_{11} = 0.266$, $u_{12} = -0.176$, $u_{22} = -0.150$) in the model.

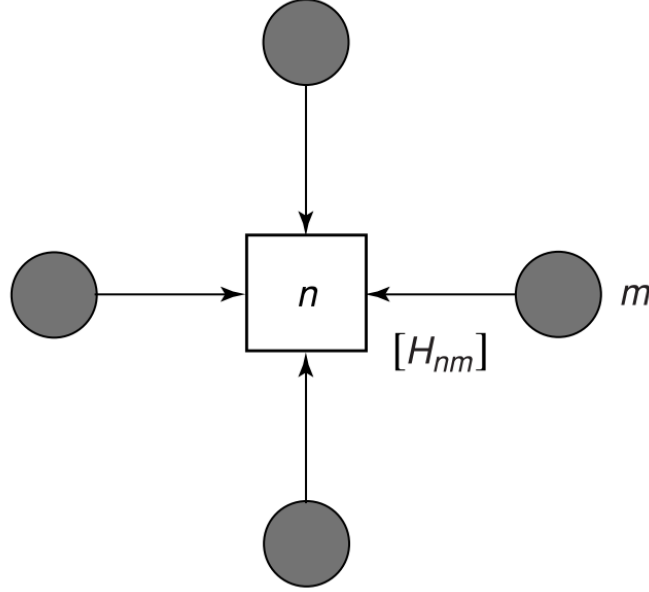


Figure 1.13 Schematic picture showing a unit cell and its neighboring unit cells [84].

1.7 Outline of the Thesis

In the chapter 2, we investigate device-to-device variability of metal-contact MoS₂ FETs where Schottky barrier height is treated as a key device parameter that determines the overall performance of transistors. Although metal contacts are widely used to realize present-day nanoscale devices, doped contacts can also be used in TMDC FETs to enhance device performance [90][91]. Therefore, we perform a comparative study of MoS₂ FETs with metal and doped contacts to see how much performance can be improved by using ideal Ohmic contacts. The short-channel effects will be discussed by scaling the channel length (L_{ch}) from 20 nm down to 4 nm. Finally, we discuss an alternative way to reduce device-to- device variability in MoS₂ FETs.

In principle, multilayer MoS₂ can be more advantageous than single layer MoS₂ for a variety of photodetector applications due to the higher density-of-states [69] and the wider spectral response from ultraviolet (UV) to near-infrared (NIR) [92]. Therefore, in chapter 3, optoelectronic design of multilayer MoS₂ phototransistors is focused to enhance photocurrent and demonstrate an alternative approach to obtain high photoresponsivity using indirect-bandgap multilayer MoS₂. Unlike the previous multilayer MoS₂ phototransistors with global bottom-gate structures, fabricated multilayer MoS₂ phototransistors in a patterned local bottom-gate TFT configuration [93] are investigated to achieve giant improvement in photoresponse. It is reported that, for light with a wavelength of 532

nm, the phototransistor based on mechanically exfoliated MoS₂ flakes exhibits high responsivity (up to 342.6 AW⁻¹ at 2 mWcm⁻¹) and linear relationship between photocurrent and incident power density over a wide range of optical power. In particular, the inclusion of an ungated region in the MoS₂ channel increases responsivity by 3 orders of magnitude as compared to that of global-gate multilayer MoS₂ phototransistors from the previous study [92]. To analyze these experimental results, comprehensive simulations are described based on optical absorption, transmission probability, and transistor current equations.

Chapter 4 is about the effects of negative differential resistance (NDR) in output characteristics for monolayer MoS₂ FETs. By using TNN TB method as introduced in section 1.5.2, transport properties of monolayer n-type MoS₂ are investigated by using full-band ballistic quantum transport simulation. As a result, it shows typical I_D - V_G characteristics similar to fabricated FETs based on monolayer MoS₂ whereas NDR effects are observed in I_D - V_D curve, which results in negative output conductance g_d that should be considered seriously for circuit applications. These characteristics was previously observed in a simulation method using an atomistic TB basis of maximally localized Wannier functions (MLWFs) orbitals [94].

As future work from this, not only intrinsic unity current gain frequency and unity power gain frequency, f_t , f_{max} , respectively, will be calculated, but also extrinsic f_t and f_{max} , will be investigated in presence of contact resistance, R_c . After that, dependence of RF characteristics on channel length of FETs and equivalent oxide thickness (EOT) of gate oxide will be investigated.

Chapter 2

Contact-Dependent Performance Variability of Monolayer MoS₂ Field-Effect Transistors

By self-consistent quantum transport simulations, this chapter is devoted to contact-dependent performance variability of monolayer MoS₂ field-effect transistors. Like other nanoscale devices, most MoS₂ FETs are demonstrated by using metal contacts, and the metal-semiconductor interface significantly affects the overall device characteristics. In principle, Schottky barrier (SB) height (Φ_{Bn}) can be obtained by the difference of metal work function and semiconductor electron affinity, but recent experiments have revealed that although each metal provides different contact properties, actual Φ_{Bn} in MoS₂ FETs cannot be determined accurately from the theoretical estimate [95]. On the other hand, even with the same metal contacts, totally different device characteristics were observed in MoS₂ FETs, which implies that even state-of-the-art MoS₂ transistors cannot avoid device-to-device variability due to the non-uniformity of the channel material as well as the quality of contacts [90]. Therefore, device-to-device variability of metal-contact MoS₂ FETs on Schottky barrier height is investigated. Also device-to-device variability of non-ideal doped-contact MoS₂ FETs is compared with the counterpart of metal-contact MoS₂ FETs. After that, short channel effect is studied by varying channel length from 4 nm to 20 nm.

2.1 Simulation Setting and Device Structure

Transport properties of MoS₂ FETs are simulated using the non-equilibrium Green's function (NEGF) formalism with an effective mass approximation [84]. Analytical summation of transverse momentum modes within the first Brillouin zone calculates charge densities and currents [96]. (See Refs. [84] and [60] for equations.) The charge density and the electrostatic potential are self-consistently calculated until converged as introduced in Section 1.3 and 1.4. Along the transport direction ($K \rightarrow \Gamma$), the effective mass in the conduction band (E_c) of monolayer MoS₂ ($E_g = 1.8$ eV) is determined as $0.45m_0$ (m_0 being the free electron mass). The effective mass for the contact metal is $1.01m_0$ [97]. Ballistic transport is assumed due to the short channel lengths.

In this chapter, we explore n-type MoS₂ transistors [65], [98], and p-type conduction in MoS₂ [99] is beyond the scope of this study. In solving electrostatics, the Dirichlet and the Neumann boundary conditions are applied for the metal and the doped contacts, respectively, to treat different types of

contacts. The nominal device has a 10-nm channel length with a 2.8-nm-thick HfO_2 ($\kappa = 25$) bottom gate insulator. Power supply voltage of $V_{DD} = 0.5$ V is applied and room temperature is assumed.

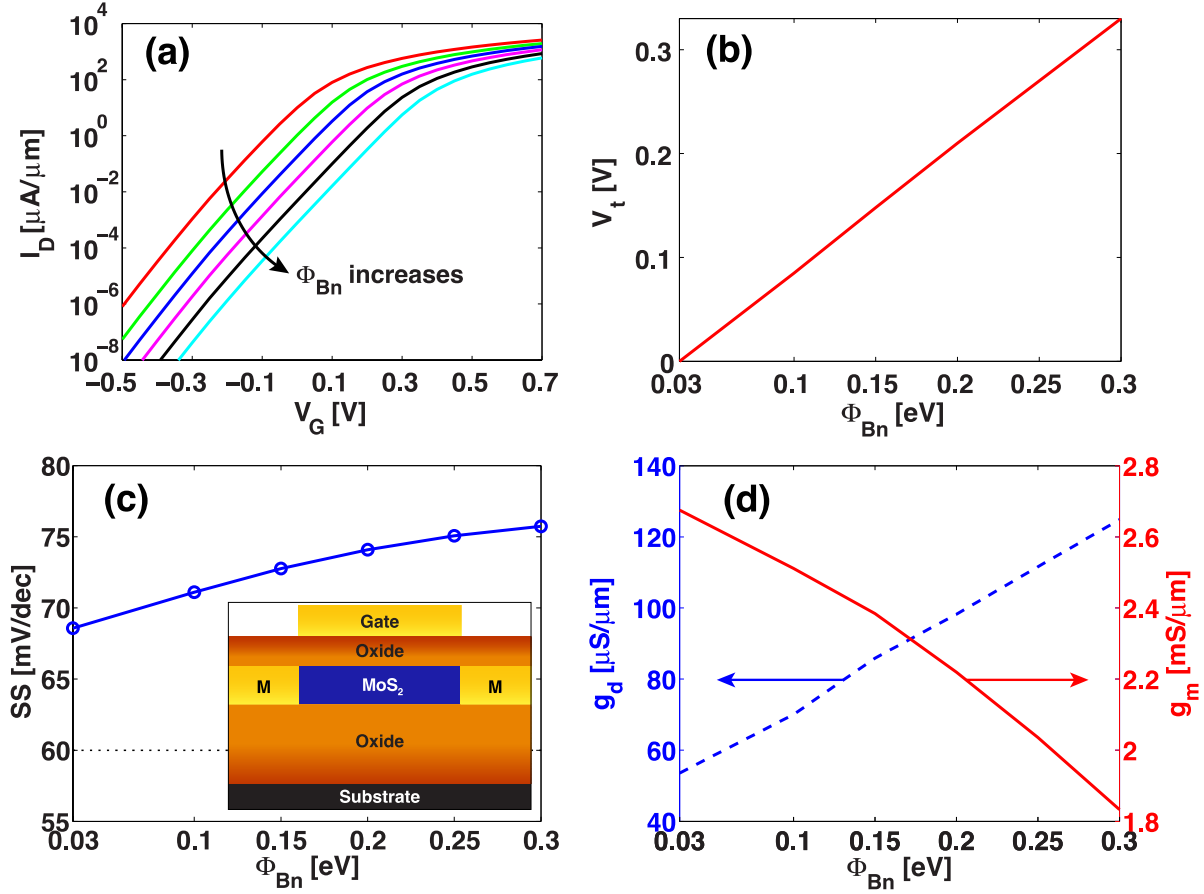


Figure 2.1 Effects of metal contact variation in MoS_2 FETs (a) I_D - V_G characteristics of MoS_2 FETs with various Schottky barrier (SB) heights (Φ_{Bn}) from 0.03 to 0.3 eV. (b) Threshold voltage (V_t), (c) subthreshold swing ($SS = \partial V_G / \partial \log_{10} I_D$), and (d) transconductance ($g_m = \partial I_D / \partial V_G$, right axis) and output conductance ($g_d = \partial I_D / \partial V_D$, left axis) as a function of SB height. The inset in (c) illustrates the structure of MoS_2 FET with metal contacts. The dotted line in (c) shows an ideal SS of 60 mV/dec for reference.

2.2 Effects of Metal-Contact Variation

First, variation of device characteristics in metal-contact MoS_2 FETs is investigated for Φ_{Bn} from 30 to 300 meV, assuming non-ideal contact properties induced by various interface conditions or defects in the channel [90], [95]. Figure 2.1(a) shows I_D - V_G curves with different SB heights, which exhibit

linear threshold voltage (V_t) shifts [Fig. 2.1(b)]. Therefore, for a fair comparison of devices with different contact properties, the same gate overdrive voltage ($V_{ON} = V_G - V_t$) is used in calculating transconductance ($g_m = \partial I_D / \partial V_G$) and output conductance ($g_d = \partial I_D / \partial V_D$), whereas subthreshold swing ($SS = \partial V_G / \partial \log_{10} I_D$) is achieved at $V_{OFF} = V_{ON} - V_{DD}$. In general, large SB height has resulted in lower device performance. By increasing Φ_{Bn} by 10 times from 30 to 300 meV, SS and g_m show relatively insignificant degradation by 10% and 30%, respectively [Figs. 2.1(c) and 2.1(d)]. However, for the same change in Φ_{Bn} , the g_d is increased significantly by 130% [Fig. 2.1(d)]. Therefore, our simulation results indicate that output characteristics can be more susceptible to non-uniform contact properties than transfer characteristics for 10-nm-channel MoS₂ FETs.

2.3 Device Characteristics of Ohmic Contact

It should be noted that, although better device performance can be achieved by using smaller Φ_{Bn} or ensuring good metal-semiconductor interface property, there exists an intrinsic limit imposed by a heterojunction. This is why significant efforts have been made to reduce contact resistance by doping 2D materials [67], [91], [100]. In this section, we will investigate how much performance can be improved in MoS₂ FETs if ideal Ohmic contacts are realized in place of metal contacts. The device structure shown in Fig. 2.1(c) remains the same except that doped contacts are used in source and drain. In this comparative study, the minimal Φ_{Bn} of 30 meV is used for metal-contact FETs [95], and a source/drain doping density of $N_d^+ = 2 \times 10^{20} \text{ cm}^{-3}$ is used for doped-contact FETs [91]. For a fair comparison, gate metal work function was modulated in each device so that a common I_{OFF} of $1.7 \times 10^{-3} \mu\text{A}/\mu\text{m}$ can be achieved at $V_G = 0 \text{ V}$ (V_{OFF}) and ON state is defined at $V_G = 0.5 \text{ V}$ ($V_{ON} = V_{OFF} + V_{DD}$). The I_{OFF} is carefully defined such that both devices have at least 5 orders of magnitude in I_{ON}/I_{OFF} and the I_{ON} of a few hundred $\mu\text{A}/\mu\text{m}$ ($507 \mu\text{A}/\mu\text{m}$ for the device with doped contacts; $303 \mu\text{A}/\mu\text{m}$ for the device with metal contacts).

Transfer characteristics of those devices are compared in Fig. 2.2(a) where an MoS₂ FETs based on doped contacts shows 67% higher I_{ON} , 48% larger g_m , and smaller SS (63 mV/dec) than its metal-contact counterpart. Although Fig. 2.2(a) is shown within the voltage window of V_{DD} , we have simulated transfer characteristics for a wide voltage range to plot I_{ON} vs. I_{ON}/I_{OFF} [Fig. 2.2(b)]. In general, large I_{ON} as well as large I_{ON}/I_{OFF} are preferable for transistor operations, and our simulations show that doped contacts can provide larger I_{ON}/I_{OFF} than metal contacts by one order of magnitude for the same I_{ON} of $500 \mu\text{A}/\mu\text{m}$ with $V_D = 0.5 \text{ V}$.

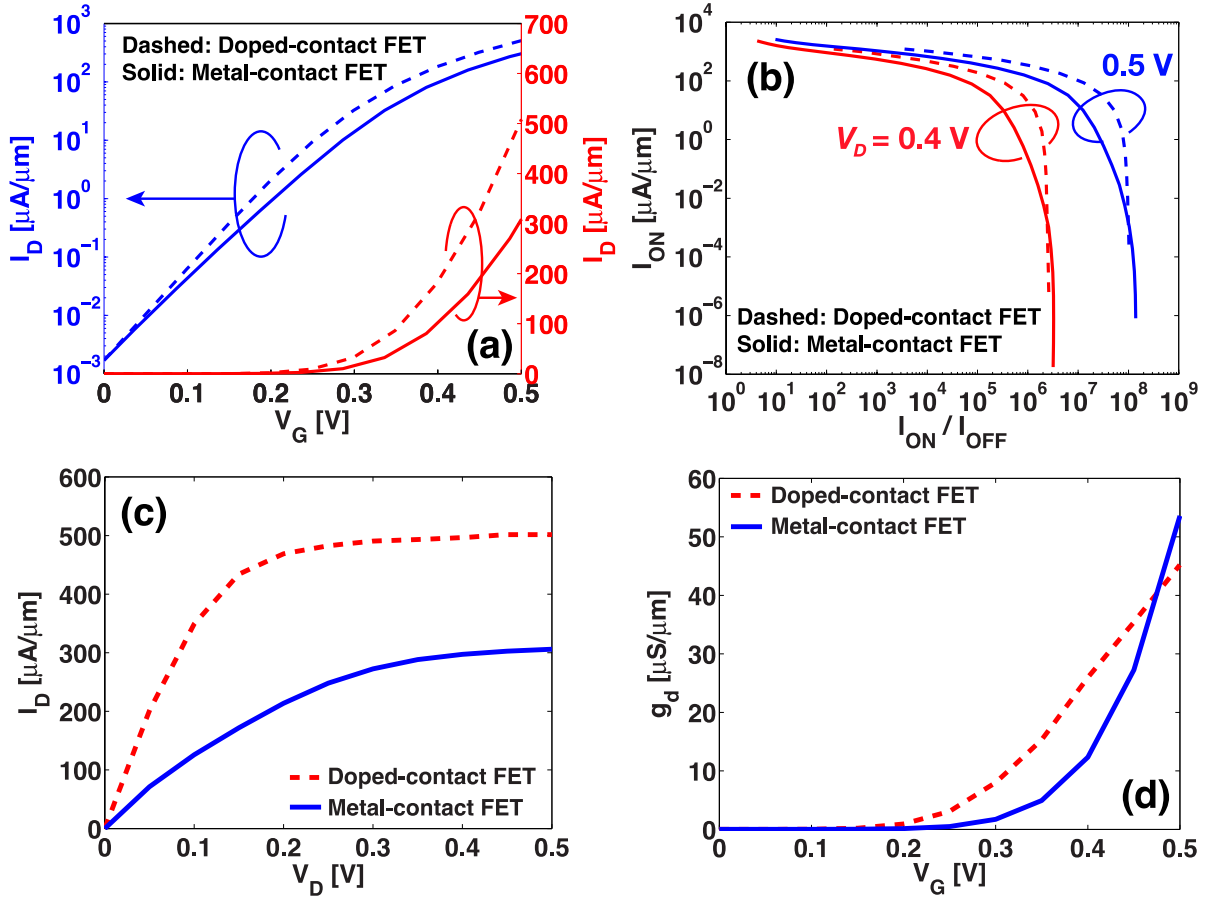


Figure 2.2 Performance improvement with ideal Ohmic contacts (a) I_D - V_G characteristics after gate work-function engineering, by which V_{OFF} (where a common I_{OFF} of $1.7 \times 10^{-3} \mu\text{A}/\mu\text{m}$ is achieved for both devices) was shifted to $V_G = 0$ V, for a fair comparison of different devices. Plots are shown on a logarithmic scale (left axis) and a linear scale (right axis). (b) I_{ON} versus I_{ON}/I_{OFF} with $V_D = 0.4$ and 0.5 V. (c) I_D - V_D characteristics at ON state ($V_{ON} = V_{OFF} + V_{DD} = 0.5$ V). (d) Output conductance at $V_D = 0.5$ V for various gate voltages.

Output characteristics of the same devices are also compared at $V_G = 0.5$ V [Fig. 2.2(c)] where both devices show clear saturation behaviors (g_d being 45 and $54 \mu\text{S}/\mu\text{m}$ for doped-contact and metal-contact FETs, respectively). Figure 2.2(d) depicts the variation of g_d with gate voltages. Doped contacts provide a smaller g_d than metal contacts by 17% at $V_G = 0.5$ V, but the opposite is observed at lower gate voltages ($V_G < 0.45$ V). This indicates that, although thermionic current is more susceptible to the variation of V_D with doped contacts than with metal contacts at low gate voltages,

the Schottky barrier thickness is more sensitive to the V_D variation at high gate voltages than the top of the barrier in doped-contact FETs.

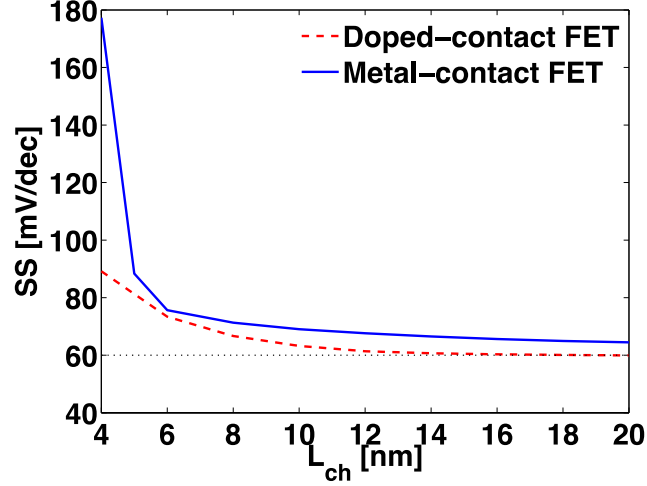


Figure 2.3 Subthreshold swing for various channel lengths (L_{ch}) from 4 to 20 nm. The dotted line is the same as in Fig. 2.1(c).

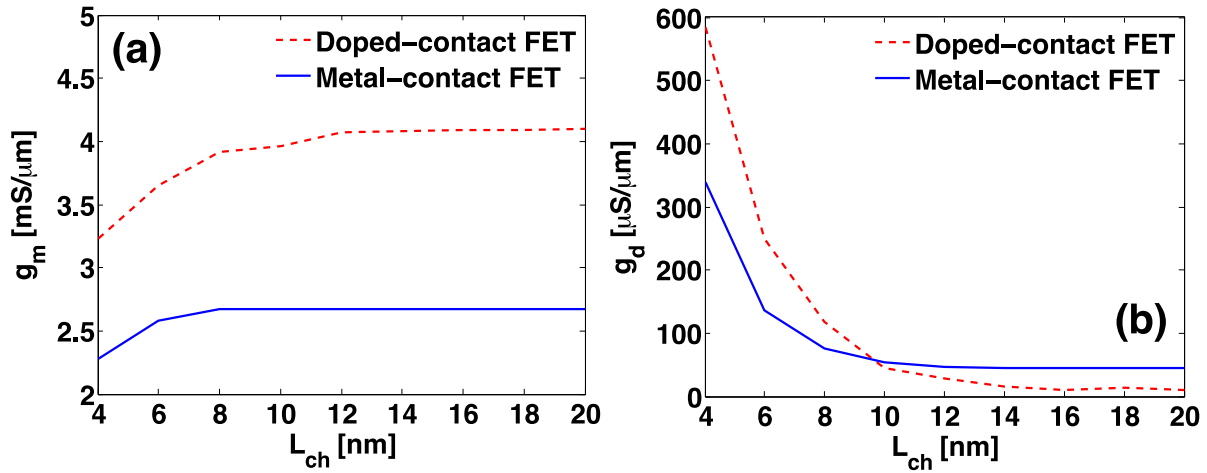


Figure 2.4 (a) Transconductance and (b) output conductance as a function of L_{ch} .

2.4 Scaling of Channel Length

Characteristics of nanoscale devices are affected by various device parameters, among which channel length is one of the most critical factors to determine the overall device performance. Here we investigate short-channel effects by varying the L_{ch} from 4 to 20 nm (Fig. 2.3). In comparing devices

with different channel lengths, SS is calculated at the bias point where the common I_{OFF} ($1.7 \times 10^{-3} \mu A/\mu m$) is achieved, whereas common ON currents (determined from the nominal 10-nm-channel devices) are used independently for doped-contact and metal-contact FETs to determine ON voltages where g_m and g_d are calculated. The doped-contact FETs have steeper subthreshold slope and larger g_m than metal-contact counterparts for the entire channel lengths simulated. Especially for the L_{ch} shorter than 5 nm, doped contacts are more robust in terms of switching: SS of the 4-nm doped-contact FET is 90 mV/dec whereas the metal-contact counterpart loses the gate control significantly, showing a large SS of 177 mV/dec. In both devices, the degradation of g_m with a 4-nm channel is relatively insignificant (15–20% less as compared to that in long-channel devices). While the trend of g_d shown in Fig. 2.4(b) clearly indicates short-channel effects for sub-10 nm channel in both devices, the g_d of metal-contact FETs is less susceptible to the channel length scaling than that of doped-contact FETs.

N_d^+ (cm^{-3})	SS (mV/dec)	I_{ON} ($\mu A/\mu m$)	I_{ON}/I_{OFF}	g_m (mS/ μm)
1×10^{20}	62	533	4.1×10^5	4.1
2×10^{20}	63	507	3.0×10^5	4.0
3×10^{20}	64	483	2.4×10^5	3.8

Table 2.1 Device parameters of MoS₂ FETs with different doping densities in source and drain.

		SS (mV/dec)		g_m (mS/ μm)	
		Mean	Standard Deviation	Mean	Standard Deviation
Single-point variation	Higher N_d^+	63.0	0.052	3.933	0.045
	Lower N_d^+	63.1	0.048	3.937	0.009
Random variation at 10 different positions		63.1		3.97	

Table 2.2 Device parameters of MoS₂ FETs with non-uniform doping in the source region.

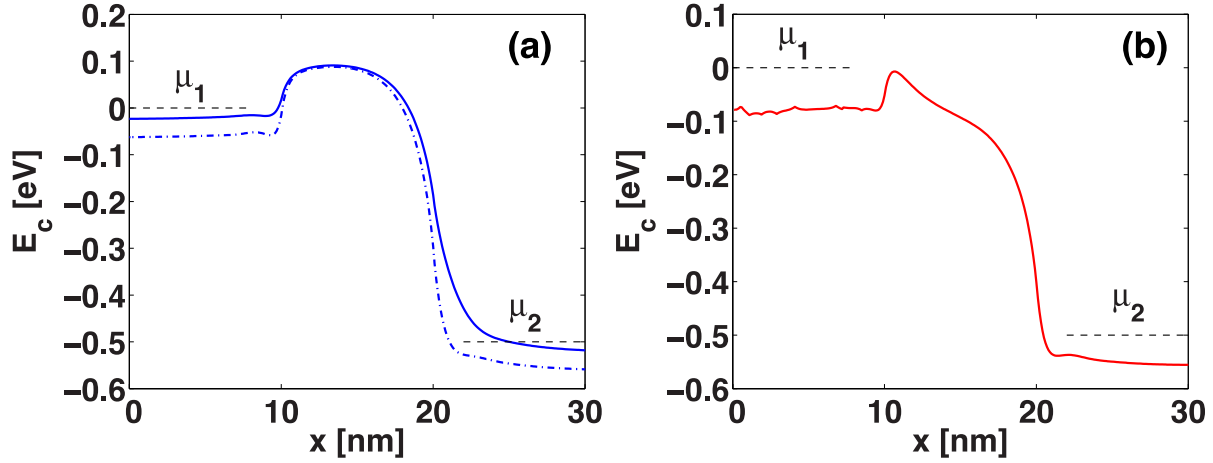


Figure 2.5 Effects of source/drain doping density (N_d^+) variation in doped-contact MoS₂ FETs
(a) Conduction band (E_c) profile at $V_G = 0.25$ V with N_d^+ of 1×10^{20} (solid line) and $2 \times 10^{20} \text{ cm}^{-3}$ (dash-dot line). (b) E_c at the ON state where doping fluctuation is treated in the source region by using higher ($2.76 \times 10^{20} \text{ cm}^{-3}$) and lower ($1.23 \times 10^{20} \text{ cm}^{-3}$) doping concentrations at 10 different random positions. The average doping concentration is kept as $2 \times 10^{20} \text{ cm}^{-3}$ in the source. $\mu_{1,2}$ are chemical potentials at the source and the drain, respectively.

2.5 Effects of Doping Density Variation

Next, we examine the effect of source/drain doping density by varying N_d^+ from 1×10^{20} to $3 \times 10^{20} \text{ cm}^{-3}$ for doped contacts. Device parameters calculated with different doping densities are shown in TABLE I. Our simulation results indicate that, unlike the impacts of Schottky barrier in metal-contact FETs, the effects of different source/drain doping densities are negligible ($< 10\%$) and the intrinsic device performance remains virtually intact for the range of N_d^+ considered in this study. This is due to the fact that carriers flowing over the barrier in the channel are controlled by the gate in the same way regardless of source/drain doping density as can be seen in Fig. 2.5(a). So far, we have considered only uniform doping concentration. In practice, however, non-uniform doping can be expected particularly for nanoscale devices due to random dopant fluctuation [101]. Here, we investigate the effect of such non-uniform doping in the source region for the following two cases: (i) single-point variation with higher ($N_d^+ = 2.76 \times 10^{20} \text{ cm}^{-3}$) or lower ($N_d^+ = 1.23 \times 10^{20} \text{ cm}^{-3}$) doping density (assuming one more or one less electron per 200-nm width); and (ii) random variations at 10 different positions along the source. For the single-point variation, the non-uniform spot is varied from one end to the other within the source. Mean and standard deviation of SS and g_m

are calculated for 10 different cases (TABLE II), which show minor performance variation by the non-uniform doping at a single point. For the random doping variation at 10 different positions inside the source, the conduction band profile is shown in Fig. 2.5(b). Even in this case, SS and g_m remain almost intact (TABLE II). Therefore, it is expected that doped-contact FETs are more robust against the non-ideality of contacts than metal-contact FETs.

2.6 Schottky Barrier Thickness Variation

Before we conclude, it will be instructive to discuss an alternative way to suppress the performance variability in MoS₂ FETs particularly with metal contacts. Recent experiments demonstrated large improvement of performance including field-effect mobility in Schottky-contact MoS₂ FETs by doping the channel material [100]. This is attributed to the reduced contact resistance as we demonstrate in Fig. 2.6 using our simulations where the Schottky barrier thickness is drastically reduced by increasing doping in the channel region. It should be noted that, if contact resistance becomes very small due to the thinness of barrier, the device performance will not be affected significantly by the SB height and, therefore, metal-contact MoS₂ FETs become less susceptible to contact variations.

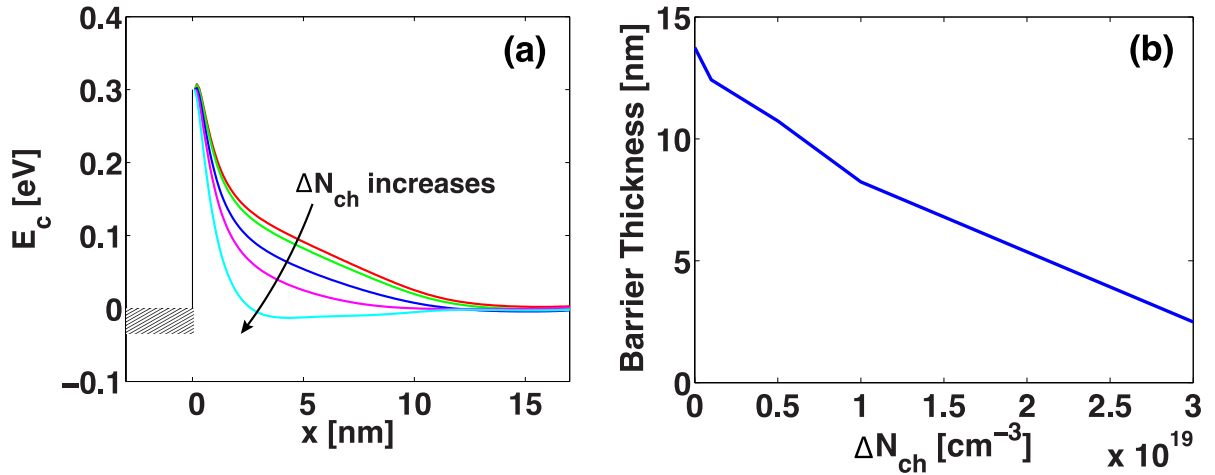


Figure 2.6 Schottky barrier thickness variation with different channel doping (a) Conduction band profile for different doping increment in the channel ($\Delta N_{ch} = 0, 1 \times 10^{18}, 5 \times 10^{18}, 1 \times 10^{19}, 3 \times 10^{19}$ cm⁻³). Gate underlap (ungated channel) is introduced at $0 \leq x \leq 10$ nm to examine the effect of channel doping. (b) Barrier thickness as a function of ΔN_{ch} at the energy of 4 meV above the source Fermi level (where the maximum contribution to the current is achieved for the largest doping density).

Chapter 3

High Photoresponsivity in Multilayer MoS₂ Phototransistors

Recently, thin-film transistors (TFTs) using single layer or multilayer MoS₂ exhibited higher responsivity [74], [92], [102], [103] than that of graphene TFTs in phototransistors [104], presenting great potential for photodetector applications. The responsivity, defined as the ratio of photocurrent flowing in a detector to incident optical power, is a primary figure of merit in photodetectors. To enhance the responsivity of MoS₂ phototransistors, various approaches have been suggested including the improvement of mobility [102], contact resistance [102], and interfacial quality of MoS₂ phototransistors [103], or the use of multijunction heterostructures with amorphous silicon [105] or graphene [106], [107]. As a result, the responsivity of single layer MoS₂ phototransistors has been drastically increased from 7.5 mA/W [74] to 880 A/W [102]. Meanwhile, the responsivity of multilayer MoS₂ phototransistors (~100 mA/W) [92] has remained much lower than that of single layer MoS₂ photodevices, mainly due to the indirect nature of the bandgap in multilayer MoS₂ and low quantum efficiency compared to single layer MoS₂ [56]. However, there are more advantageous properties in multilayer MoS₂ than single layer MoS₂, for example, higher density of states and wider spectral response. Thus, this chapter shows how much photocurrent and photoresponsivity is boosted in newly designed optoelectronic structure of indirect-bandgap multilayer MoS₂.

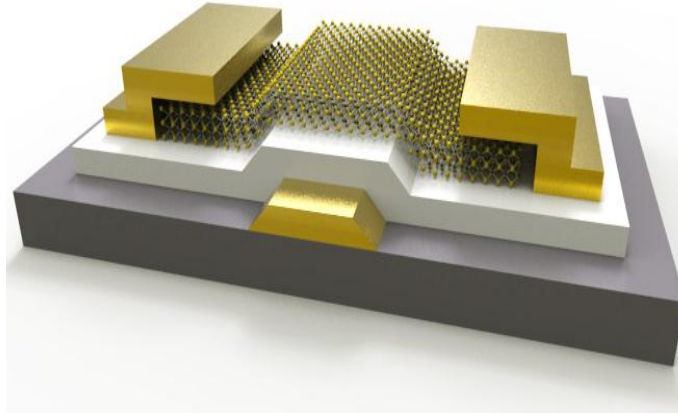


Figure 3.1 Multilayer MoS₂ phototransistor in a local bottom-gate structure [93].

3.1 Device Structure

Device structure configured by Kim *et al.*[93] is shown in Fig 3.1 which is 3D section view of a phototransistor with a local bottom gate on a glass substrate. The samples fabricated and

experimented by professor Kim's group in Kyung Hee University in Korea has a similar configuration to that of a commercially used bottom-gate inverted-staggered device. The typical structure contains gate metal underneath the active layer and source/drain contacts on the top. However, unlike the conventional structure, the gate length is shorter than the channel length. This "local" bottom-gate structure leads to a gate underlap, which is a non-overlapped (ungated) region between the gate and the channel. Goal of this chapter is to analyze optoelectronic characteristic of this device.

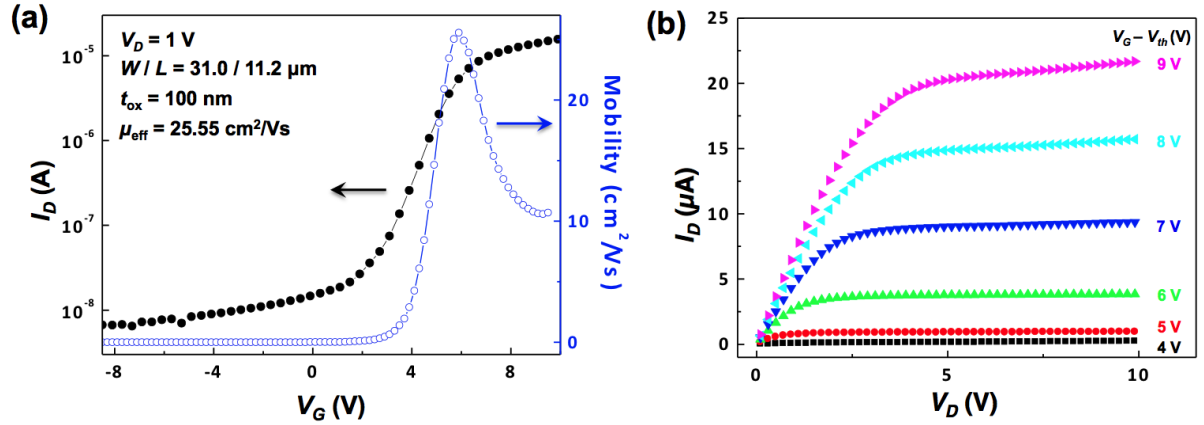


Figure 3.2 Device characteristic of local bottom-gate multilayer MoS₂ phototransistor (a) Transfer characteristic (I_D - V_G) curve and field-effect mobility at $V_D = 1$ V. (b) Output characteristic (I_D - V_D) curves of the same device with different gate biases ($V_G - V_{th} = 4, 5, 6, 7, 8$, and 9 V) [93].

3.2 Device Characteristics

Before analyzing the optoelectronic behavior of a multilayer MoS₂ phototransistor under incident light, current-voltage (I - V) characteristics measured by Kim *et. al.* [93], with local bottom-gate MoS₂ TFT (channel length $L = \sim 11.2$ μm , device width $W = \sim 31.0$ μm , and gate length = ~ 8.8 μm) in dark state, should be identified. The thickness of multilayer MoS₂ channel and gate oxide thickness (t_{ox}) are 80 nm and 100 nm, respectively. Fig. 3.2(a) shows the measured transfer (I_D - V_G) characteristics in logarithmic scale and the extracted mobility value of the TFT. The maximum transconductance ($g_m = \left. \frac{\partial I_D}{\partial V_G} \right|_{V_D=1V}$) of 4.38 μS , a field-effect mobility ($\mu_{eff} = Lg_m / (WC_{ox}V_D)$) of 25.55 $\text{cm}^2/\text{V}\cdot\text{s}$, and I_{ON}/I_{OFF} of $\sim 10^3$ are observed. Here, an atomic layer deposited aluminum oxide (Al₂O₃) gate insulator exhibits excellent insulating properties (leakage current = ~ 50 pA at $V_G = 5$ V) and offers well-

controlled electrostatic potential with a relatively small gate-bias modulation. Fig. 3.2(b) shows the output (I_D - V_D) characteristics of the same device. Titanium/Gold (Ti/Au) source and drain electrodes provide excellent Ohmic contacts to the multilayer MoS₂, resulting in the linear behavior at low drain voltages, and the fully saturated current at high V_D . Although its local bottom-gate MoS₂ phototransistor shows the device characteristics of conventional n -type long-channel TFTs in dark state, its performance is not as good as that of other reported global-gate multilayer MoS₂ TFTs due to the underlap in the local-gate geometry.

3.3 Modeling and Simulation for Contacts Properties

Transmission probability was calculated by using the non-equilibrium Green's function (NEGF) method within the effective mass approximation [84]. Coherent transport is assumed as the length and the width (W/L) are treated in the classical current equation. The effective mass of 0.5 was used for multilayer MoS₂ [108]. In general, good contact properties are essential to ensure large drive current, especially for the transistors with significant gate underlap regions. We have estimated the degradation of current due to the gate underlap as

$$I_{dark}^{local} = I_{dark}^{global} \times \overline{Tr}^{underlap} \quad (3.1)$$

where I_{dark}^{local} and I_{dark}^{global} are dark current for local-gate and global-gate structure, respectively, and $\overline{Tr}^{underlap}$, average transmission probability through the underlap region, is introduced to consider current degradation due to the gate underlap. First, $I_{dark}^{global} = 3.00 \times 10^{-5}$ A is obtained from the current equation for the conventional long-channel devices in the linear region with the following parameters: field-effect mobility of 100 cm²/V·s [69], oxide capacitance of 6.20×10^{-4} F/m², device width of 31.0 μm, channel length of 11.2 μm at $V_{ON} = V_G = 6.5$ V (threshold voltage, $V_{th} = 4.75$ V) and $V_D = 1$ V. Since the measured current value of our local-gate device structure at the same bias condition ($V_G = 6.5$ V and $V_D = 1$ V with $V_{th} = 4.75$ V) is 3.31×10^{-6} A, we estimate $\overline{Tr}^{underlap}$ to be 0.11 and the current is smaller than that of an ideal global-gate TFT by roughly 1 order of magnitude. In order to understand this current degradation, transmission probability through the gate underlap at on state assuming two different contact conditions was calculated as shown in Fig. 3.3(a). First, a relatively large Schottky barrier height ($\Phi_{Bn} = 100$ meV) was defined and a transmission probability through the triangular tunnel barrier in the gate underlap region is calculated by varying the length of underlap from 1 Å to 1 μm (squares in Fig. 3.3(b)). The Schottky barrier height ($\Phi_{Bn} = 100$ meV) is assumed for tunneling where the transmission probability is calculated at the energy level of 10 meV below the

top of the Schottky barrier. Our simulation result shows that transmission probability becomes zero at 1- μm gate underlap, which clearly indicates that current cannot flow through the large Schottky barrier if the underlap length is significant as in our device (1.41 μm). Obviously, this is not the case that we have observed in the experimental report. Next, we defined a small Schottky barrier ($\Phi_{\text{Bn}} = 10$ meV) assuming that carrier transport is near-thermionic rather than tunneling as illustrated at the bottom in Fig. 3.3(a). The transmission probability is calculated again at the top of the barrier for the same range of gate underlap. To be specific, this is calculated at the energy level of 10 meV above the chemical potential of the source (μ_s). The energy level of the largest contribution to the current is carefully selected by comparing transmission probability weighted by $(f_s - f_D)$ where $f_{1,2}$ are the Fermi function at source and drain, respectively. For the ungated channel region, linear potential drop is assumed [109]. The result shows that, under this condition, the current decreases gradually as the underlap length increases, but will not be completely diminished even with 1- μm gate underlap. This indicates that a normal TFT operation is still possible with the local-gate structure even though current level will be reduced as compared to that of global-gate TFTs. Therefore, the analysis, along with the linear I_D - V_D behavior at low drain voltages, implies that the Schottky barrier height of our local bottom-gate MoS_2 TFT is negligibly small and Ohmic contact has been achieved.

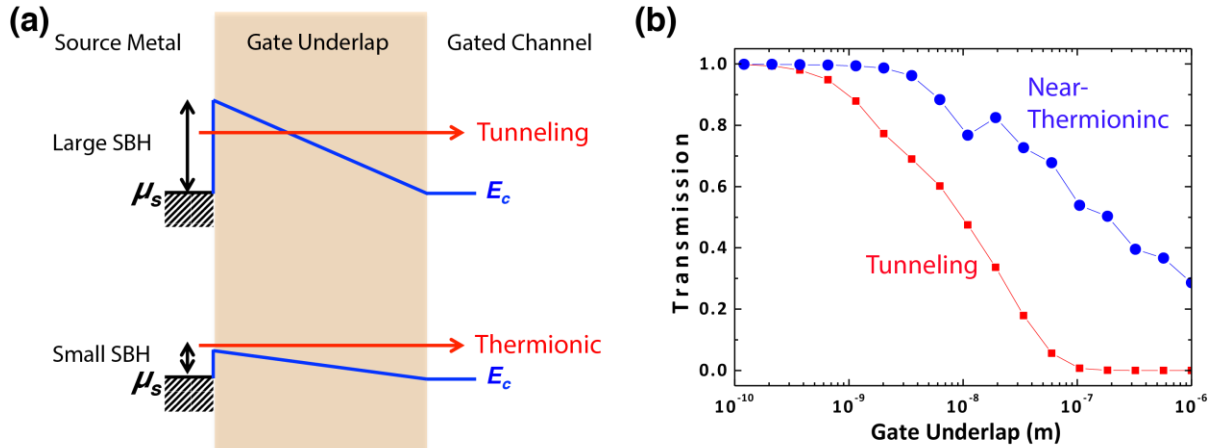


Figure 3.3 (a) Tunneling (top) and near-thermionic emission (bottom) through the gate underlap with a large and a small Schottky barrier height (SBH), respectively, at the metal- MoS_2 interface. μ_s is the chemical potential at the source and E_c is the conduction band edge of MoS_2 . (b) Transmission probability at various lengths of gate underlap for tunneling (squares) and near-thermionic emission (circles). If current is observed in the device with a gate underlap of 1 μm , it means that thermionic emission is dominant since tunneling would be impractical.

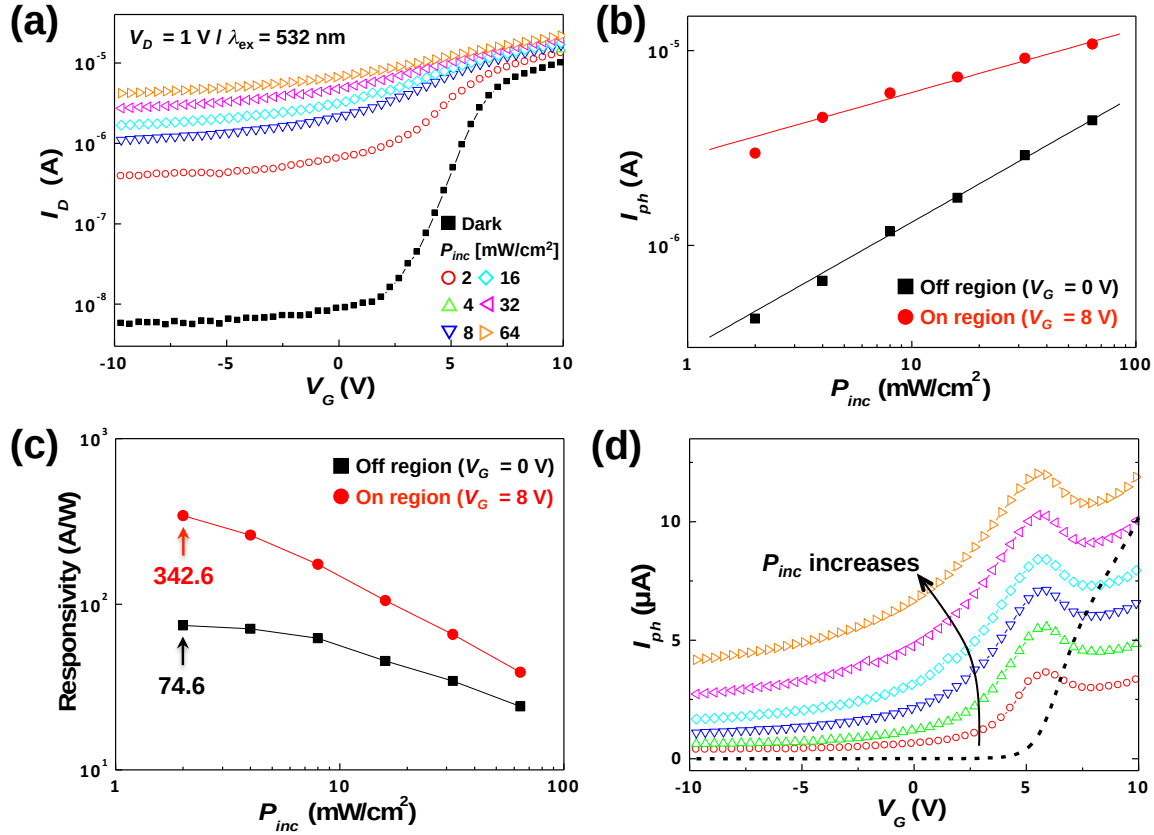


Figure 3.4 Photoresponsive behavior of a multilayer MoS₂ local bottom-gate phototransistor. (a) Comparison of transfer characteristics (I_D – V_G) under dark (solid symbol) and light condition (open symbols) with various incident optical power densities ($\lambda_{ex} = 532$ nm, $P_{inc} = 2, 4, 8, 16, 32$, and 64 mW/cm²). (b) Photocurrent ($I_{ph} = I_D - I_{dark}$) and (c) responsivity as a function of incident power in logarithmic scale, obtained in off ($V_G = 0$ V) and on ($V_G = 8$ V) region. (d) Photocurrent at various gate voltages for the same conditions of illumination as in Fig. 3.4(a) (open symbols). Dark current is also shown as a reference (dashed line). (e) Log-scale photoswitching behavior at three different light intensities (2, 4, and 6 mW/cm²) at a wavelength of 638 nm ($V_G = -5$ V and $V_D = 1$ V). Photocurrent modulation is induced by the laser, which is switched on and off every 20 s. (f) Linear-scale photocurrent in (e) during one cycle of light illumination at 6 mW/cm².

3.4 Photoresponse Amplification in Local Bottom-gate MoS₂ TFT

Then how much incident light amplify photoresponsivity of this TFT in [93]? Fig. 3.4(a) is experimental result that shows how transfer characteristics of the local bottom-gate MoS₂ TFT are influenced by incident light for the various power densities (P_{inc}) from 2 to 64 mW/cm² at a wavelength of 532 nm and drain voltage of 1 V. Under the illumination of light at 64 mW/cm², the current has been increased by 3 orders of magnitude in the off state and by 2.5 times in the on state, respectively. While photoresponsive characteristics are demonstrated only at the off state in the previous multilayer MoS₂ TFT with a conventional global-gate geometry [92], the local-gate device in [93] shows the significant enhancement of current with light both at on and off states. Fig. 3.4(b) presents photocurrents ($I_{ph} = I_D - I_{dark}$) as a function of power density at off ($V_G = 0$ V) and on state ($V_G = 8$ V). This device shows the excellent linear response of photocurrent to the logarithmic change of optical power, indicating that the local bottom-gate TFT can be used for sensing photons. Responsivity, $R = I_{ph} / P_{inc}$ is also calculated, and the maximum value of 342.6 A/W is obtained at 2 mW/cm² in the on state (Fig. 3.4(c)). Note that this is remarkably higher by more than 3 orders of magnitude than the previously reported value for multilayer MoS₂ TFTs. The large enhancement of photoresponsivity can be also observed in Fig. 3.4(d), where photocurrent is plotted for different optical power densities (open symbols) and dark current is also shown as a reference (dashed line). Unlike the previous multilayer MoS₂ phototransistors, the photocurrent of this new device in the on state is as comparably large as the dark current, which is achieved by using the local bottom-gate structure.

To characterize the photoswitching behavior of the local bottom-gate MoS₂ TFT, the time-resolved photore-sponse was measured as shown in Figure 3.5(a). The measurement was carried out at $V_G = -5$ V and $V_D = 1$ V under 638 nm laser at three different incident power densities (2, 4, and 6 mW/cm²). As the illuminating light is switched on and off at an interval of 20 s (a period of 40 s), photocurrent is generated and recombined in accordance with the illumination. A nearly identical response is observed for multiple cycles, exhibiting the reproducibility and the robustness of our local bottom-gate transistors. Figure 3.5(b) shows photocurrent measured during one cycle of light modulation in linear scale. Although an accurate response time is not measurable within our experimental setup, the overall photo switching characteristics demonstrate the potential of our local bottom-gate MoS₂ TFTs for highly sensitive photodetector applications.

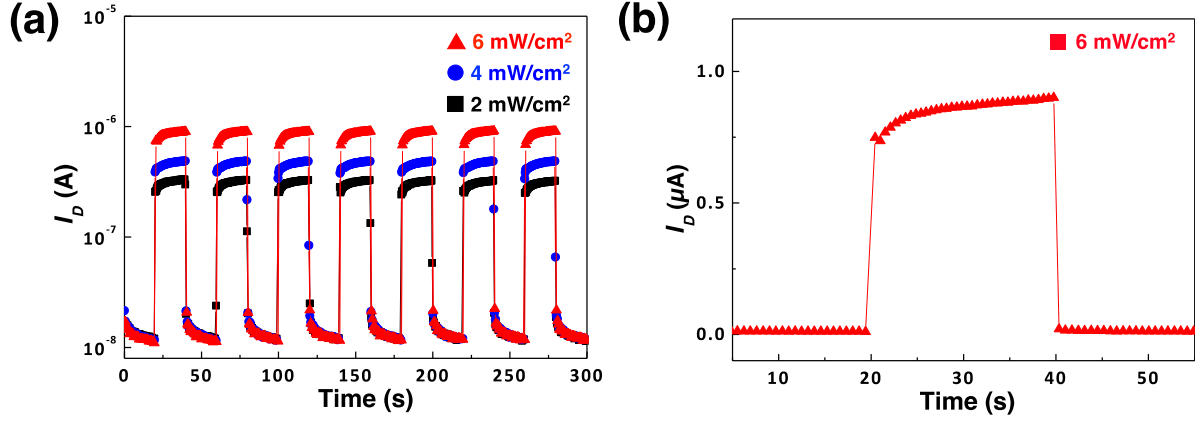


Figure 3.5 (a) Log-scale photoswitching behavior at three different light intensities (2, 4, and 6 mW/cm²) at a wave-length of 638 nm ($V_G = -5$ V and $V_D = 1$ V). Photocurrent modulation is induced by the laser, which is switched on and off every 20 s. (b) Linear-scale photocurrent in (a) during one cycle of light illumination at 6 mW/cm².

3.5 Analysis for Photoresponse Amplification

Next, to understand the photoresponse amplification using the local-gate structure in MoS₂ TFTs, we have plotted photocurrent at 2 mW/cm² at $V_G = 0$ V (Fig. 3.6(a)), which shows a non-linear behavior to the applied V_D due to parasitic resistance in the channel region. If the gate underlap is negligibly small or a global-gate structure is used, it would show a linear response to V_D (*e.g.*, see Fig. 4(c) in Ref. [92]) following the current equation based on optical absorption as

$$I_{ph} = 2e \frac{P_{inc}(1 - e^{-\alpha d})}{h\nu} \tau \mu \frac{W}{L} V_D \quad (3.2)$$

where e is elementary charge, α and d are absorption coefficient and thickness of multilayer MoS₂, respectively, $h\nu$ is energy of incident photon, τ is average carrier lifetime, and μ is mobility of carriers. However, in our local bottom-gate MoS₂ TFT, such linearity is broken due to the asymmetric barrier in the underlap region as illustrated in the inset of Fig. 3.6(a). In particular, holes generated by illuminating light encounter the large tunnel barrier imposed by the gate underlap and they must overcome that large barrier to reach the source (dashed arrow in the inset) whereas electrons can move toward the drain relatively unhampered. Therefore, holes are trapped in the channel region and this local accumulation of holes can reduce the potential barrier for electrons (the top in Fig. 3.6(b)),

resulting in the significant increase of thermionic current even with a relatively small optical power (also see Fig. 3.4(a)). In fact, I_{ph} of our local-gate MoS₂ TFT in the off state is significantly larger than that of a global-gate structure by more than 2 orders of magnitude for the similar conditions. Moreover, I_{ph} becomes even larger at higher gate voltages (Fig. 3.4(d)). This is due to the fact that, as V_G increases, the barrier for the holes will be gradually decreased (as shown in the bottom in Fig. 3.6(b)). In addition, the dark on current of local-gate TFTs can be smaller than that of global-gate devices for the same channel length due to the series resistance that we have discussed earlier. To sum up, (i) enhanced I_{ph} in the off state, (ii) reduced barriers at larger gate voltages, and (iii) suppressed dark on current are all supportive of photoresponsivity in the on state in our local bottom-gate MoS₂ TFT and, thereby, the large value of 342.6 A/W could be obtained using our unique device structure.

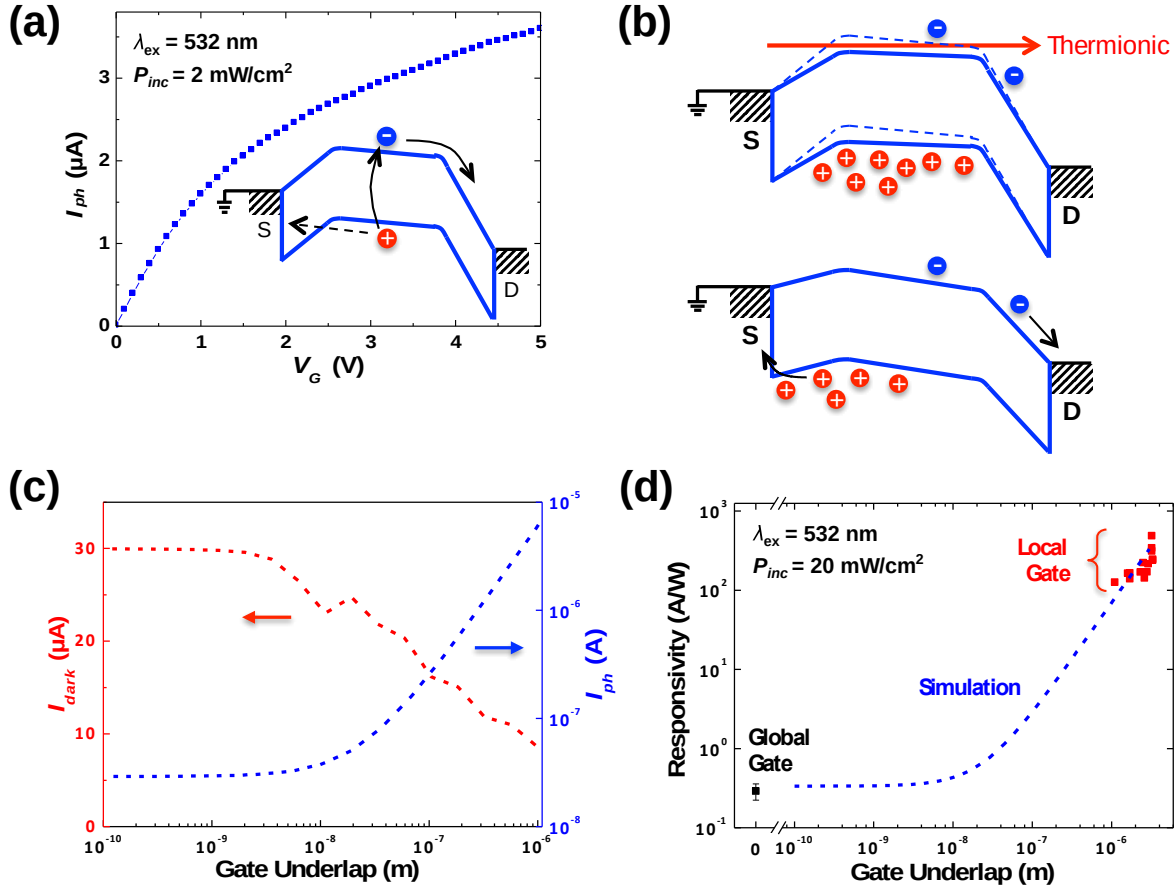


Figure 3.6 (a) Photocurrent at various drain voltages. Inset: Energy band diagram in the off state. (b) Top: Energy band diagram showing significant accumulation of holes due to the large gate underlap, which reduces the potential barrier for electrons from dashed to solid lines, resulting in the increase of thermionic current. Bottom: Energy band diagram at an increased gate voltage where the barrier for the hole will become smaller as V_G increases, leading to larger photocurrent. (c) Dark current (left axis) and photocurrent (right axis) as a function of gate-underlap length. (d) Photoresponsivity for a various lengths of gate underlap. A cross symbol shows the value from our experiment. The responsivity from the previous multilayer MoS₂ global-gate phototransistor is also shown, which is close to the simulation result with the shorter lengths of gate underlap we considered.

3.6 Modeling and Simulation for Dependence of I_{ph} on Scaling of Gate Underlap

It might be instructive to investigate how the length of gate underlap affects photoresponsivity in the local-gate MoS₂ TFTs. We have performed comprehensive simulations, which show that, while dark on current can be gradually reduced with gate underlap following the Eq. (3.1) (Fig. 3.6(c) with the left axis), photocurrent will increase significantly as shown in Fig. 3.6(c) with the right axis. In this simulation, the photocurrent is calculated as

$$I_{ph} = I_{EHP} + 2 I_{off}^{global} \times \exp\left(\frac{e\Delta V_{off}}{mk_B T}\right) \quad (3.3)$$

where I_{EHP} is current due to the generation/recombination of electron-hole pairs by illuminating light, I_{off}^{global} is dark current at off state with global-gate geometry, $e\Delta V_{off}/m$ is potential energy lowering due to the hole accumulation under the illumination of light, m is body-effect coefficient, k_B is Boltzmann constant, T is temperature, and a factor of 2 comes from our experimental observation to treat the increase of photocurrent in the on state (see Fig. 3.4(d)) for a fixed optical power. Off current of the global-gate transistor (I_{off}^{global}) is calculated by the current equation for the conventional long-channel devices in the subthreshold region with the following parameters: $\mu_{eff} = 100 \text{ cm}^2/\text{V}\cdot\text{s}$, $C_{ox} = 6.20 \times 10^{-4} \text{ F/m}^2$, $W = 31.0 \text{ }\mu\text{m}$, $L = 11.2 \text{ }\mu\text{m}$ at $V_{OFF} = V_G = -1 \text{ V}$ ($V_{th} = 4.75 \text{ V}$) and $V_D = 1 \text{ V}$. The body-effect coefficient of the device is calculated from the measured subthreshold swing (SS) as $m = (SS/2.3) \times (e/k_B T) = 21$. I_{EHP} is treated invariant for different gate voltages at a given optical power and $I_{EHP} = 5000 I_{off}^{global}$ is assumed. The effect of potential barrier lowering is treated by $e\Delta V_{off}/m$ where ΔV_{off} is changed from 0 to 8 V as the length of gate underlap increases from 1 Å to 3 μm.

As the gate underlap increases, holes will be accumulated more and the barrier will be reduced, resulting in larger $e\Delta V_{off}$. Photoresponsivity is calculated from this photocurrent at 20 mW/cm^2 in Fig. 3.6(d), which exhibits the trend that the responsivity significantly increases with the gate underlap for the length longer than 10 nm. Statistical distribution of our experimental photoresponsivities for 28 representative multilayer MoS₂ phototransistors is also shown by solid symbols, which is close to the simulation result. Therefore, our experimental data and simulation results provide comprehensive pictures on giant photoamplification in indirect-bandgap multilayer MoS₂ phototransistors based on local bottom-gate multilayer MoS₂ system.

Chapter 4

Negative Differential Resistance (NDR) of Monolayer MoS₂ FETs

4.1 State-of-art NDR FETs

Differential resistance is defined as the derivative of voltage with respect to the current. In I–V curve, it is inverse slope at a point.

$$r_{diff} = \frac{dv}{di} \quad (4.1)$$

Negative slope (declining to the right) is negative differential resistance (NDR), i.e., $\Delta v/\Delta i < 0$. Therefore, NDR is a characteristic of devices in electric circuits, resulting in a current decrease with increasing voltage across it.

There are several research groups that have reported NDR in graphene FETs (GFETs). One of them showed that bottleneck effect by the graphene Dirac point induces NDR in GFETs by using NEGF simulation [110]. Only when the gate voltage generates polarity configuration of n-p-n and p-n-p, NDR is occurred in the GFETs simulations. They also investigated RF performance of monolayer GFETs using simulations at the NDR bias region. Even though maximum oscillation frequency is decreased by about 1.5-3 times, a voltage gain larger than 10 can be achieved [111].

For the MoS₂ FETs, Chang *et al.* not only reported analysis of NDR in MoS₂ FETs [94] but also compared TMDC based n-type/p-type FETs. The 3-nm channel monolayer MoS₂, MoSe₂, and MoTe₂ n-type MOSFETs are also simulated to investigate transport properties. With the fact that underlaps of the channel material brings fair subthreshold swing, the dependence of NDR in output characteristics on material orientations was discussed and reported.

4.2 Simulation Method

Self-consistent simulation with NEGF and the Poisson equation is set and utilized as in chapter 2, except the Hamiltonian matrix, H . TNN TB model is employed, which gives more rigorous band structure of monolayer MoS₂ and the parameters are obtained by fitting the first-principle energy bands as mentioned earlier in section 1.6. In this device, double gate geometry with n-type single layer MoS₂ is exploited to ensure a good electrostatic control. Channel, source, drain length are all 15 nm and source/drain doping density is $4 \times 10^{20} \text{cm}^{-3}$ to make Fermi level, μ_S , be located at around

0.1 eV higher than E_c of the source. Like chapter 2, it has 2.8-nm-thick HfO_2 ($\kappa = 25$) bottom and top gates insulator. Applied power supply voltage is $V_{DD} = 0.5$ V.

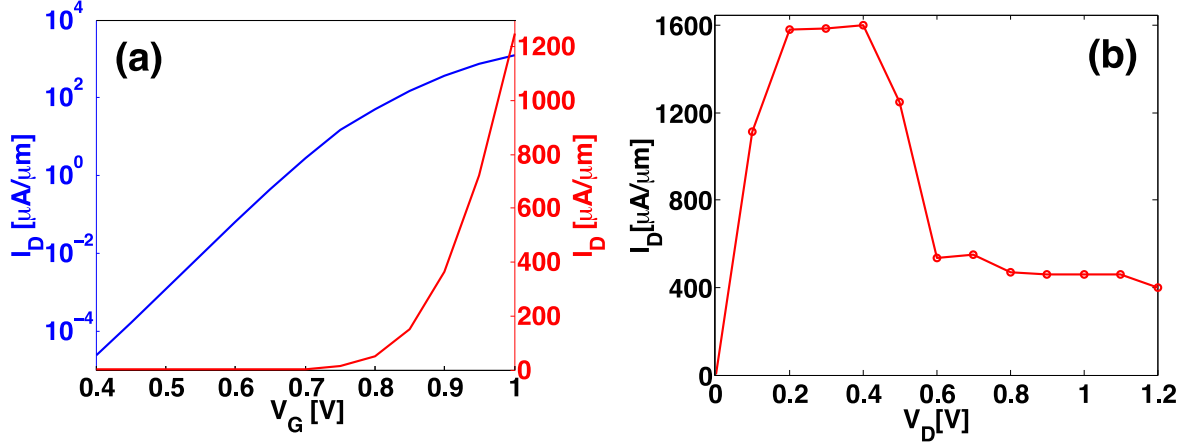


Figure 4.1 Device Characteristics of monolayer MoS_2 base on TNN TB Hamiltonian (a) I_D - V_G characteristics. Plot is shown in a logarithmic scale (left axis) and a linear scale (right axis). (b) I_D - V_D characteristics at ON state ($V_{ON} = 1.0$ V).

4.3 Analysis of NDR Effects

As shown in [94], reason why I_D - V_D current is degraded at high V_D is due to the number of mode difference between conduction band in drain region and that in source region at the same energy level. The electrons that contribute to total current are injected from the source to channel near the bottom of the conduction band. Not like effective mass or graphene E - k bandstructure, there exist satellite valleys in TMDC bandstructures. Therefore, both global and local minima in conduction band should also be considered since capturing the injected electron at the energy level in the drain region is occurred at moderate drain voltages. Let's see band structure in transport direction considering the rectangular 1st BZ shown in Fig. 4.2(a). This TNN TB model bandstructure of MoS_2 monolayer is plotted with a super cell including 4 atoms when $k_y = 0$ and $-\pi/a_x < k_x < \pi/a_x$ where a_x is lattice constant of MoS_2 [89]. There are two incoming states, all in the lowest lying conduction band with open square symbols. This curve is located on source and drain potential profile through $V_D = 0.5$ V (see Fig. 4.2(b)) and the solid black line indicates energy level which has the highest transmission along entire region. When around $0.2 \text{ V} < V_D < 0.5 \text{ V}$, since number of outgoing mode including same band in the drain, which captures electrons from incoming mode in source is four, transmission by this transport leads to large total current shown as high flat current level in I_D - V_D plot

in the V_D region. However, when V_D reaches 0.5 V, the number of available outgoing mode is reduced to two that is not matched with k value of incoming mode and this results in smaller transmission [94].

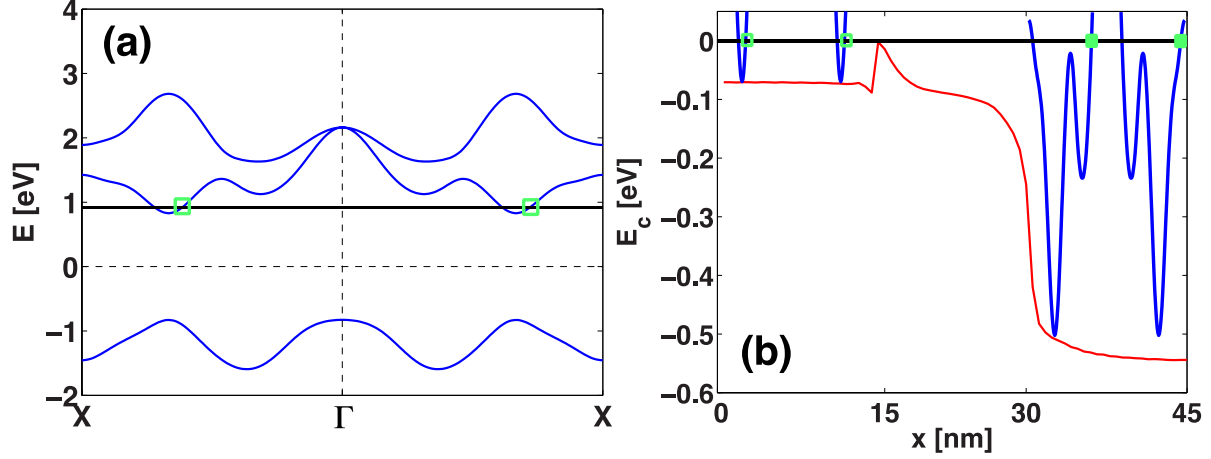


Figure 4.2 (a) Bandstructure of TNN TB Hamiltonian of monolayer MoS₂ of rectangular BZ at $k_y = 0$ and $-\pi/a_x < k_x < \pi/a_x$. (b) Conduction band profile of the MoS₂ FET with bandstructure on it at source and drain region.

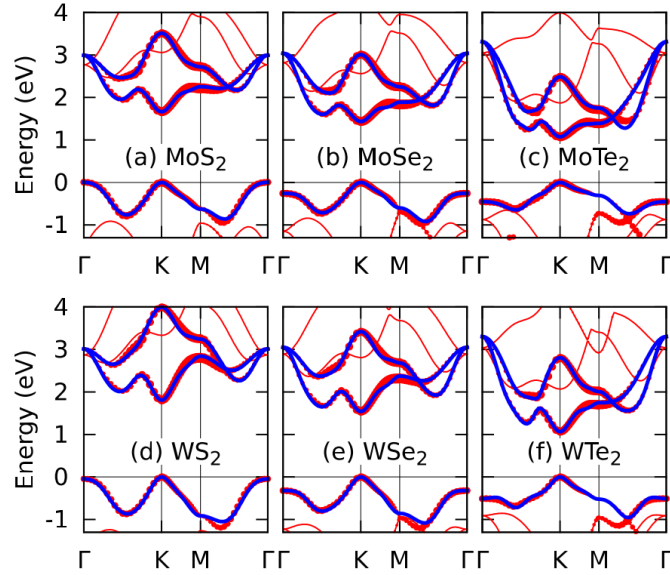


Figure 4.3 Energy bands from the TNN TB model (blue or dark curves) of MX₂ monolayers compared with the First Principle ones (red or gray curves and dots) [89].

In this subsection, we can confirm that TNN TB model describes more precise behaviors of electrons in the channel material. By using the model we observed the NDR effect in output characteristics above $V_D = 0.5$ V drain region due to decreasing number of outgoing mode of bandstructure and thereby reduced transmission between mismatched modes.

Chapter 5

Conclusion and Future Work

5.1 Conclusion

In summary, the performance variability of MoS₂ FETs with different contacts is investigated by means of quantum transport simulations. Our simulation results reveal that the variation of Schottky barrier in MoS₂ FETs can affect output characteristics more significantly than transfer characteristics. If ideal Ohmic contact is realized in place of metal contact, I_{ON} and g_m can be improved by 67% and 48%, respectively, and I_{ON}/I_{OFF} can be increased by one order of magnitude for the same drive current. While doped-contact FETs are more robust than metal-contact devices at sub-10-nm channel length in terms of switching characteristics, larger output conductance of doped-contact FETs indicates that short-channel effects can be more significant. Although the doped contacts can also provide robustness against contact variations in MoS₂ FETs, channel doping in metal-contact devices can effectively reduce contact resistance and suppress device-to-device performance variability.

Multilayer MoS₂ phototransistors with local bottom-gate structures was also presented, in which a gate-controlled region was connected in-series to gate underlap (ungated) regions. Compared with the conventional global bottom-gate structure, our local-gate MoS₂ phototransistor showed outstanding photoresponse. Specifically, the significant enhancement of photocurrent was observed in both on and off states, and the maximum responsivity of 342.6 A/W was achieved at 2 mW/cm². The simulation revealed that the gate underlap region plays an essential role in enhancing the optoelectronic behavior of indirect-bandgap multilayer MoS₂ phototransistors. It is expected that the same strategy can also be applicable to other material systems including monolayer MoS₂ for photoresponsivity amplification through proper engineering of Schottky barrier and gate underlap. The excellent photoresponsive characteristics of our devices suggest that high-gain photodetectors based on multilayer MoS₂ can be realized by engineering optoelectronic device design. Combined with large-area synthesis of MoS₂, the unique architecture in the local bottom-gate multilayer MoS₂ phototransistors can enrich optoelectronic applications such as touch screen panel, image sensor, and communication devices.

Lastly, NDR effect that current decreases with increasing drain voltage is investigated. Even though this TNN TB single layer MoS₂ FET show decent I_D - V_G characteristics, degraded output current is exhibited in I_D - V_D characteristics at $V_D > 0.5$ V. It is revealed that unique shape of

bandstructure of MoS₂, inclusion of satellite valley beyond the conduction band minima, causes reduced transmission of injected electrons from source to drain.

5.2 Future Works

Effects of L_{ch} on f_t should be investigated considering scattering regime since scattering offset the short channel effect and f_t is affected by the effect in graphene FETs according to the [112]. Therefore, new f_t will be calculated with $g_m^{scattering} (= g_m^{ballistic} \times (\lambda/\lambda + L_{ch}))$, where λ being the scattering mean free path has channel length dependence.

Secondly, gate dioxide is HfO₂ whose relative permittivity is 25 in our nominal device. Since f_t depends on EOT as shown in graphene FETs [112], simulation will be conducted with various EOTs and how EOT scaling affects on f_t will be investigated. It is expected that g_m would be increased with small EOT due to better electrostatic control, but rate of increase of C_g will be the key factor that determines trend at the various range of EOTs.

Maximum oscillation frequency (f_{max}), that is a frequency at which the power gain becomes unity, is also significant figure of merit for RF applications. The intrinsic f_{max} can be described as this [113]:

$$f_{max} = \frac{f_T}{2\sqrt{g_d R_g + 2\pi f_T C_{gd} R_g}} \quad (5.1)$$

and gate resistance, R_g [113], is

$$R_g = \alpha R_{sh} \frac{W}{L_{ch}} \quad (5.2)$$

where $R_{sh} = 0.33 \frac{\Omega}{\square}$ is the sheet resistivity of metal gate, $\alpha = 1/3$ is a constant for distributed gate resistance. In fig 4.1(b), this monolayer MoS₂ FETs simulation with TNN TB Hamiltonian shows negative differential resistance effect in output characteristics, which contain V_D region where g_d is negative value. At high drain voltage region, current value is degraded to approximately 1/3 of the higher flat region at $0.2 \text{ V} < V_D < 0.4 \text{ V}$. Since this negative g_d , which should be calculated at $V_{DD} = V_D = 0.5 \text{ V}$, could results in complex number of f_{max} , Eq. (5.1) cannot be employed in this situation. Therefore, derivation of a new f_{max} equation counting on NDR should be investigated.

Additionally, for extrinsic f_t and f_{max} , effect of a series contact resistance will be considered. Contact resistance, R_C , equally divided and connected to source and drain terminals. To embed this effect in our simulator, the semianalytical model is applied by this self-consistent calculation [110].

$$\mu_{S'/D'} = \mu_{S/D} \mp q \frac{R_C}{2} I \quad (5.3)$$

where upper/lower sign indicates for source/drain. Original Fermi level $\mu_{S/D}$ is iteratively replaced with $\mu_{S'/D'}$ subtracting or adding applied voltage across R_C to Fermi energy level of source and drain, respectively.

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