A Numerical Study of Si-TMD Contact with n/p Type Operation and Interface Barrier Reduction for Sub-5 nm Monolayer MoS₂ FET

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Abstract

An atomic-scale numerical study of Si contact with transition metal dichalcogenides (TMD) semiconductor materials is proposed by first-principles simulation for the first time. The monolayer MoS₂ channel can be operated as both of n- and p-type FET by properly doping Si S/D to adjust the TMD channel potential. The gradient MoS_x junction of dichalcogenide vacancies enables Si-MoS₂ contact resistance lower than 100Ω-μm for interface Schottky barrier height reduction. The compact Si-MoS₂ interface study can potentially provide monolayer TMD contact design guideline for the sub-5 nm TMD FET fabrication technology.

I. Introduction

Traditional Si channel field effect transistors (FET) have faced physical limitation in nano-scale transistor, there are many alternative novel materials were proposed to meet the channel scaling of Moore's law [1]. First monolayer MoS₂-FET was proposed in 2011 [2] since advanced 2D semiconductor material is an ideal channel material for its unique sub-nm monolayer ultra-thin body [3] and good transport property at extremely small thinness [4]. Moreover, there are many lately published results [5-9] demonstrated TMD-FET have great potential in sub-10nm channel length FET application (Table 1). However, TMD contacts heterogeneous integration still is a big challenge in n- and p-channel formation and contact resistance reduction. In this paper, the numerical study of TMD contacts between monolayer MoS₂ and bulk Si with unique contact techniques was presented in atomic scale first-principles simulations. The design of TMD FET structure for CMOS compatible process is still lack. From this work, we also show that the n/p FET operation very well at the same TMD channel layer with properly n/p type doping at Si S/D contact for sub-5nm channel MoS₂ FET, which could be compared with our experimental result[7]. We can also predict a minimum achievable contact resistance well below 100Ω-μm with dichalcogenide vacancies in the gradient Si-MoS_x junction.

II. Simulation Approach

This numerical DFT calculations made use of Atomistix ToolKit (ATK2015). The whole process is designed by Fig1. Firstly, one may build the interfacial structure of MoS₂-Si with assistance of minimum strain package in ATK, which greatly shorten calculation time of the unit cell geometry optimization. To sample the K-space of contact region, 9x13x1 k points were adopted, higher k points is required for repetition bulk calculation. The density mesh grid cut-off follows previous study [9] with 200Ry and an acceptable geometry optimize force as 0.05eV/Å. The Hartwigsen-Goedecker-Hutter (HGH-T8) pseudo-potential basis is chosen for closely matching experimental value of band gap 1.8eV in MoS₂. To describe many particle internal interaction and van der Waals interactions between layers, an exchange and correlation interactions of the generalized gradient approximation (GGA) and Grimme DFT-D3 are used here. Substituting all above parameters into Kohn-Shan Equation leads to a self-consistent calculation of electron density. Once the charge density is converged with minimum energy, the bulk simulation is completed, and associated physical quantities of electron density, band structure and density of state (DOS) is found. Current simulation is associated with electron transport calculation. Generally the system consisted of a central region (channel-MoS₂) and two contact (scattering in MoS₂-Si) region. Such canonical system calculation can be expanded with previously optimized bulk structure's state and using non-equilibrium Green's function (NEGF) method to calculate transmission spectrum. Once the zero-bias transmission spectrum is calculated, one may speed up finite-bias ones by initializing a new calculation from previous converged state of another. Integrating the transmission coefficient over the bias windows gives the transport current. Hence a useful MoS₂ FET based on first-principles current simulation is archived.

Many experimental literatures [1-8] demonstrated that solid CMOS processes on Si substrate can be very compatibility for sub-10 nm channel length MoS₂ FET manufacturing. Therefore, Fig. 2 (a) shows the simulated schematic of a monolayer MoS₂ FET device with Si source/drain along the channel in this work. Furthermore, to

reduce the Schottky barrier and improve Si-MoS₂ contacts, we need understand the nature of the electronic interface between bulk-Si and monolayer TMD. As shown in Fig. 2 (b) and (c), various Si-TMD contact regions are simulated with optimized unit cell of the Si-MoS₂ of M-S interface regions for n/p- channel operation and contact resistance reduction in the coming discussion. Unit cell optimizations gives the relaxed structure with minimum energy in Si-MoS₂ M-S contacts, and a realistic physical separation distance between them can be found.

III. Si-MoS₂ Contact Evaluation

A. Fermi Level Tuning by Doping Si Contact

Doping Si contact with TMD materials to adjust the channel chemical potential has been demonstrated in our previous experimental work [7]. Fig. 3(a)(b)(c) shows the band structure change of monolayer MoS₂ in TMD FET with different type dosage (n-doped:1E21, un-doped, and p-doped:1E21). From the band structure simulation result, the extrinsic dosed type of bulk Si can effectively adjust the MoS₂ Fermi level to close the conduction band by n-type Si contact or the valence band by p-type Si contact. Here, we didn't consider the interface diffusion or surface dipole formation, the band gap keeps the same value ($E_g \approx 1.8$ eV) in n- or p-type Si contact condition. The configuration of MoS₂ and Si (Fig. 3(d)) are nearly intrinsic. As connected to Si, the E_F of the Si-MoS₂ contact lies close to the conductance band of MoS₂, indicating that MoS₂-Si is n-typed contact ($\Phi_N=0.6$ eV, $\Phi_P=1.2$ eV). Work function shifts versus different type dosage are shown in Fig. 3(e). Noted that P: 1E20 makes original N-contact reversed to P-type one. The higher concentrations of 1E21 makes Φ_P drops to 0.2eV from 0.85eV. Similarly shift effect can also be observed in opposite direction of N-contact. From schematic picture of the DOS of Si-MoS₂ in Fig. 3(f). Compared to un-doped scheme (middle inset), P: 1E21 makes whole DOS profile shifted to higher level, making valence hole state dramatically increase (lower inset), and a P+ S/D contact is constructed. In contrast, N-doping yields profile moving downwards to lower energy (upper inset), forming N+ S/D contact. Fermi level tuning is also indirectly reflected on the threshold voltage change in current simulation. Compared to un-doped sampling in Fig. 4(a), dosage of 1E-19 shift the threshold voltage from 0.9 V to a lower position of 0.2 V with ON/OFF ratios exceeding $>10^4$ at source-drain voltage $V_{SD}=0.1$ V.

B. Rc Lowering by Gradient MoS_x Junction

Hydrogen treatment on TMD materials to compact Si-MoS₂ interface has been reported in our previous experimental work [7]. Fig. 5. shows the schematic of simulated Si-MoS₂ structure with dichalcogenide vacancy by Hydrogen treatments, where the replacement rate of Sulfur by hydrogen was marked with SV0, SV1, SV2 (25%, 50%, 100%). Fig. 6. (a) shows the average electron density along z

projected on the x-y plane of Si-MoS₂ contacts with and without dichalcogenide vacancy treatments. With SV2 treatment, the nearest physical distance between the Si atoms and the chalcogenide atoms is highly reduced to 1.46Å and the tunneling barrier Φ_{TB} decrease from 0.54 Ry to 0.23 Ry, as displayed in Fig. 6. (b). In fact the lower Φ_{TB} is associated with covalent bond formation. Fig. 7 shows the bond population at interface of SV2 compared to other metallic-MoS₂. Obviously dichalcogenide vacancy changes interface bonding type from ionic bond of 0.39 in Si-S to covalent bond of value 0.52 in Mo-Si, close to that in inner Mo-S and in Ti-S with 0.52 and 0.59. Table 2 benchmarks the sequence of normal industry metal contacts with MoS₂. Si-monolayer MoS₂ with dichalcogenide vacancy takes advantage of comparable tunneling barrier height and electron densities with metallic-TMD contacts. Fig. 8. list the calculated Schottky barrier height of Si monolayer MoS₂ under different dichalcogenide vacancy conditions. The dichalcogenide vacancy metalizes the contact interfacial surface, lowering the chemical potential. Hence the original n-type Si-contact was transferred into a P-type one. Note that as replacement rate $\sim 60\%$, an intrinsic-type junction takes place, indicating a bipolar transistor can be fabricated in the future. Fig. 9. compares the simulated contact resistance of un- and with SV1- Si- monolayer MoS₂. The curve clearly display the lowering tunneling barrier induced by dichalcogenide vacancy. In this case, the resistance drops from 75.3 $\Omega\cdot\mu m$ to 55.8 $\Omega\cdot\mu m$ (gain 33%) with 50% dichalcogenide vacancy process, close to the reduction of 29% in Φ_{TB} . Fig. 10 and Fig. 11 shows the output I_D-V_G and I_D-V_D curve for dichalcogenide vacancy engineer on monolayer MoS₂ FET. Both of the forward and reverse - I_{ON} current are increased, consistent with previous prediction of Φ_{TB} reduction. Moreover, a non-linear slope of Schottky contact can be displayed with I_D-V_G and I_D-V_D (Fig. 10, and 11). The dichalcogenide vacancy slightly drops Φ_P with more hole injection, and it significantly improves pMOS output current, as shown in Fig. 11.

IV. Conclusions

An atomic-scale numerical study of Si-MoS₂ contacts is proposed by the First Principle simulation for the first time. The n- or p- type channel formation by doping Si-TMD contacts and the SBH reduction of gradient MoS_x junctions can get well performance and contact in 4 nm channel length of monolayer MoS₂ FET. It points to the possibility of low nm node MoS₂ FET using Si-TMD contacts. It further shows a way to give monolayer TMD FETs a new feature of Si-TMD contacts in conventional Si process for the first time.

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Metallic	Ni	-	Au	-	WTe ₂	Si
channel	graphene	phosphorene	phosphorene	MoS ₂	MoS ₂	MoS ₂
contact	Adequate	edge contact	-	Mo vacancy	heterojunction	doping Si/ S vacancy
type	doping				n	
R _c	30 Ωμm	25 Ωμm	-	-	-	56 Ωμm
L _g	-	10.5 nm	7 nm	6.3 nm	3 nm	4 nm
transistor	n-type	n/p-type	n-type	TFET	TFET	n/p-type
reference	IEDM 2015 [12.7]	IEDM 2015 [12.1]	IEDM 2015 [12.2]	IEDM 2015 [12.4]	IEDM 2015 [12.3]	this work

Table 1. The simulated metallic-semiconductor contacts performance comparison table of novel 2D semiconductor.

Fig. 2. (a) Simulated structures of sub-5 nm channel length monolayer MoS₂ FET with (b) edge/ (c) side contacts (d) optimized unit cell of the Si-MoS₂ interface regions

Fig. 3. (a)(b)(c) Band structure of the metallic-MoS₂ interface with different type dosage in Si side contacts. (d) Bulk reference (e) Schottky barrier change vs. different doping condition, $\Phi_{SB,N/P}$ denotes n/p- barrier height for electrons/holes.

Fig. 3. (f) DOS spectra for n/p doping.

Fig. 4. The simulated I_D - V_G of 4nm channel length monolayer MoS₂ FET with (a) undoped (b) p-doping (c) n-doping Si contacts

Fig. 1. A Flow chart of simulating sub-5 nm channel length MoS₂ FET.

Fig. 5. Schematic of simulated Si-MoS₂ structure with S-vacancy.

Fig. 7. The covalent bond population at metallic-channel interface.

Fig. 8. The calculated Schottky barrier height of Si-monolayer MoS₂ under different S-vacancy treatments and other metallic-MoS₂.

Fig. 10. The simulated I_D - V_G of 4 nm channel length monolayer MoS₂ FET wi and w/o S-vacancy.

References

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Fig. 6. (a) The electron density of Si-MoS₂ contacts under S-vacancy treatments (red dashed line) (b) The roadmap of tunneling barrier and electron density under different S-vacancy process SV0,1,2 (25%, 50%, 100%).

MoS ₂ side contact benchmark							
	Ti	Au	Pd	Si	SV1	SV2	Si(edge)
$d(\text{\AA})$	1.5	2.7	2.2	2.16	1.68	1.46	1.21
$\Phi_{TB}(\text{Ry})$	0	0.6	0.2	0.54	0.38	0.23	0.25
$N(\text{Bohr}^{-3})$	0.033	0.018	0.029	0.018	0.025	0.026	0.041
Contact type	N	N	I	N	N	P	N

Table 2. The benchmark table of Si-monolayer MoS₂ with S-vacancy treatment and other low barrier metal contacts.

Fig. 9. The calculated contact resistance of Si-monolayer MoS₂ with S-vacancy.

Fig. 11. The simulated I_D - V_D of 4 nm channel length monolayer MoS₂ FET w/o and w/i S-vacancy.