EE32 Device Simulation Lab

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Lab 7: Performance Limits of Monolayer Transition Metal Dichalcogenide Transistors

The performance limits are examined using a ballistic model of the MOSFET. The initial results of effective mass and fermi energies calculated from bandgap are taken directly from [1]. They were simulated using VASP using ab-initio theory. The performance of monolayer MX_2 is then compared with Si in ballistic regime.

Introduction:

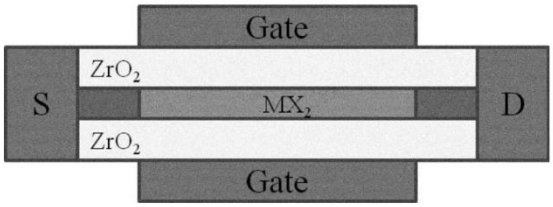


Fig. 1. Structure of a double-gate MOSFET model. The thickness of the ZrO_2 dielectric insulator $t_{ins} = 3$ nm.

We use the analytical ballistic model [2] to investigate for the performance limits of the monolayer MX_2 semiconductors as channel materials.

At zero terminal bias, the equilibrium electron density at the top of energy barrier is

$$N_0 = \int_{-\infty}^{+\infty} D(E) f(E - E_F) dE \qquad (1)$$

where D(E) is the density of states at energy E, and f(E -EF) is the Fermi distribution with EF as the Fermi level.

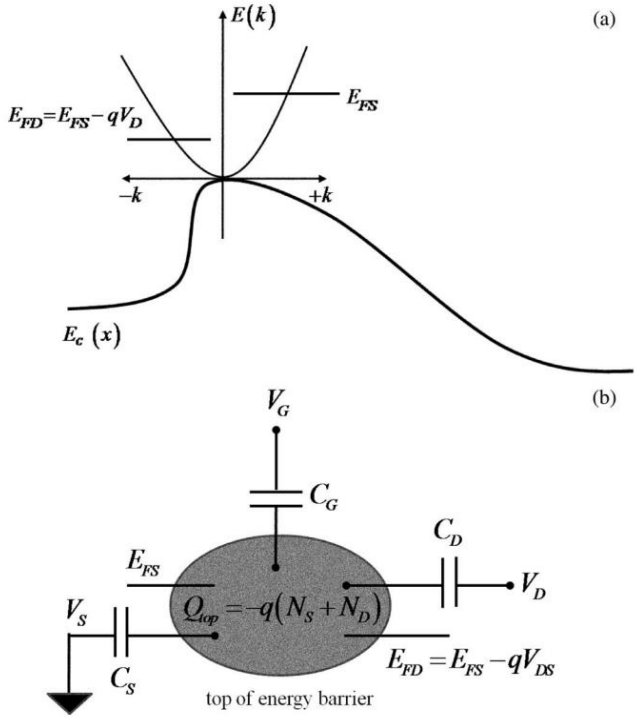


Fig. 2. (a) Illustration of the potential barrier and the source and drain Fermi energy levels. The $+k$ states are occupied by a carrier from the source, and the $-k$ states are occupied by a carrier from the drain. (b) Two-dimensional transistor model of ballistic MOSFET. The potential U_{scf} at the top of the energy barrier is controlled by the gate, source, and drain through the three capacitors, i.e., C_G, C_S, and C_D, respectively.

When the gate and drain biases are applied, the energy barrier is accordingly modulated. The positive velocity states at the top of the barrier are filled by electrons from the source, and the negative states are filled by electrons from the drain. The electron density is given by

$$N = \frac{1}{2} \int_{-\infty}^{+\infty} D(E - U_{scf}) [f(E - E_{FS}) + f(E - E_{FD})] \, dE \qquad (2)$$

Uscf is the self-consistent surface potential, which is calculated by coupling the charge density calculation to a capacitance model that describes transistor electrostatics,

$$U_{\text{scf}} = U_L + U_P \tag{3}$$

$$U_L = -q(\alpha_G V_G + \alpha_D V_D + \alpha_S V_S) \tag{4}$$

$$U_P = \frac{q^2}{C_G + C_D + C_S}(N - N_0) \tag{5}$$

The complete derivation can be looked up in [1] and [2] for the behavior of ballistic model and self consistent energy potential.

Results and Discussion:

VASP ab-initio simulation results are as shown in Table I

Since effective mass in longitudinal and traverse axis is almost same, results were quite similar too so the plots are shown for only one of them.

However, for 2-D-Si transistors, since the quantum–mechanical effect in the direction that is normal to the interface between the channel and the gate insulator is significant, the average inversion layer actually locates away from the interface, increasing the total insulator layer thickness equivalently. Also, there are no dangling bonds and, therefore, no formation native oxide on the surface of monolayer MX2.

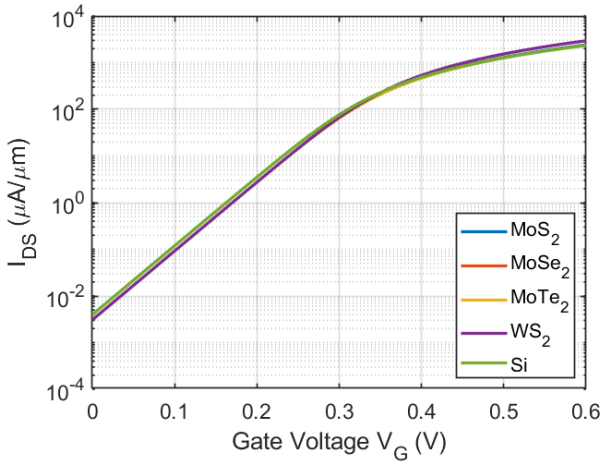
Thus effectively a thickness of 5.5nm is used for ZrO_2

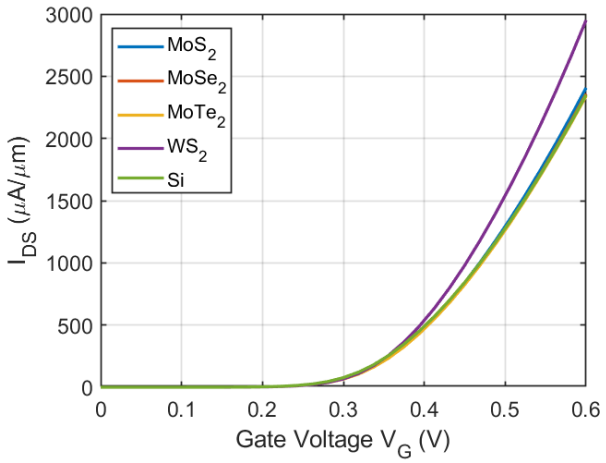
TABLE I
CALCULATED RESULTS OF MONOLAYER MX_2 USING GGA

	MoS_2	$MoSe_2$	$MoTe_2$	WS_2
a (Å)	$3.16^{(1)}$	$3.299^{(1)}$	$3.522^{(1)}$	$3.1532^{(1)}$
	$3.182^{(2)}$	$3.311^{(2)}$	$3.539^{(2)}$	$3.181^{(2)}$
c (Å)	$3.172^{(1)}$	$3.338^{(1)}$	$3.604^{(1)}$	$3.1424^{(1)}$
	$3.138^{(2)}$	$3.348^{(2)}$	$3.622^{(2)}$	$3.140^{(2)}$
E_g (eV)	$1.78^{(3)}$	$1.49^{(3)}$	$1.13^{(3)}$	$1.93^{(3)}$
m_n^x ($\times m_0$)	$0.5788^{(3)}$	$0.6059^{(3)}$	$0.6164^{(3)}$	$0.3466^{(3)}$
m_n^y ($\times m_0$)	$0.5664^{(3)}$	$0.5933^{(3)}$	$0.6033^{(3)}$	$0.3382^{(3)}$
m_p^x ($\times m_0$)	$0.6659^{(3)}$	$0.7114^{(3)}$	$0.7586^{(3)}$	$0.4619^{(3)}$
m_p^y ($\times m_0$)	$0.6524^{(3)}$	$0.6967^{(3)}$	$0.7406^{(3)}$	$0.4501^{(3)}$

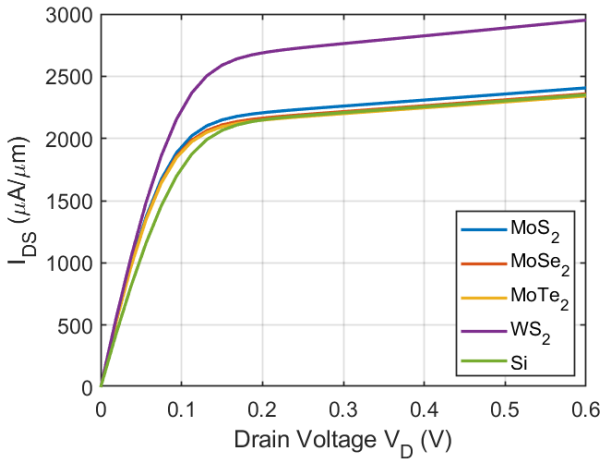
E_g is the energy band gap. $m_n^x\,(m_n^y)$ and $m_p^x\,(m_p^y)$ is the fitting effective mass for electron and hole along the $k_x\,(k_y)$ direction, respectively.
(1) Experimental data of bulk lattice parameters [7][8][22][23][24]
(2) Calculated data monolayer MX_2 lattice parameters by GGA with structure relaxation.
(3) Fitting parameters against band structure calculated by GGA with a fixed structure (using bulk lattice parameters in (1)).

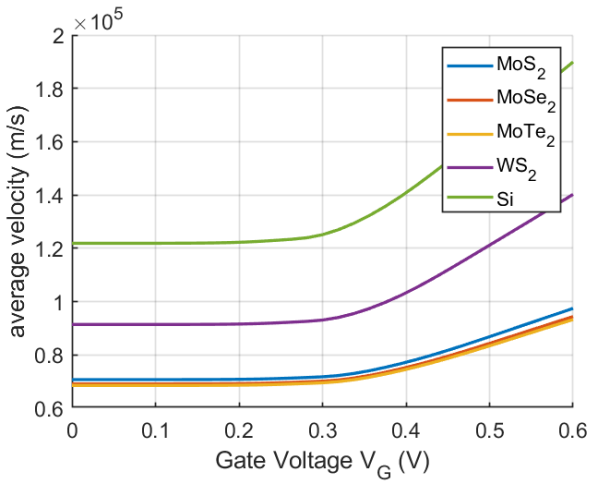
The calculated results are for n-MOSFET for V_G and V_D = 0.6V are presented as in figures below:



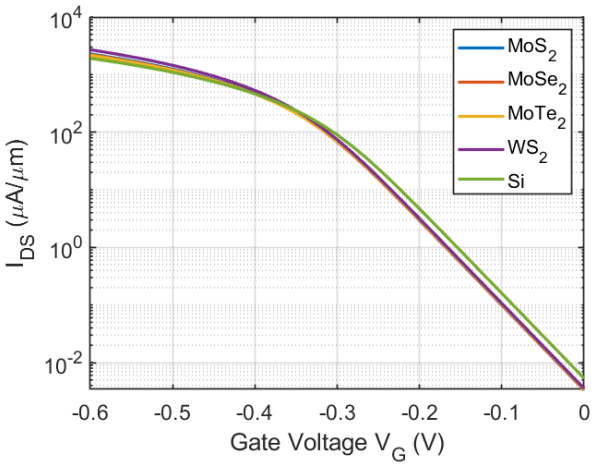


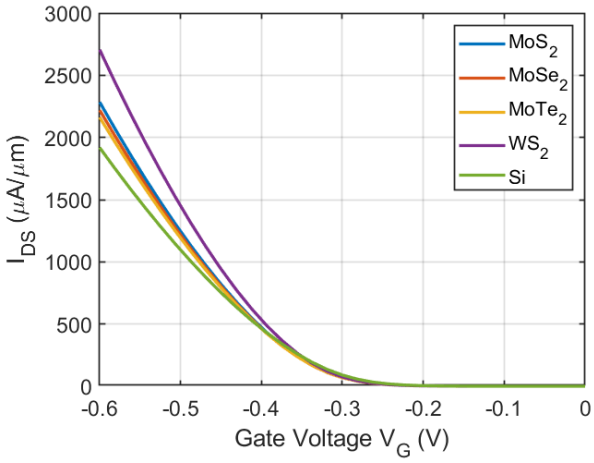
Within the ballistic regime, the monolayer WS_2 transistors have the best performance. WS_2 transistors outperform 2-D-Si transistors in terms of ON-current by about 28.3%. Due to the atomic body thickness of monolayer MX_2, transistors with these materials exhibit good gate control and result in a high ON-current. This makes monolayer MX_2 to be promising channel materials to replace Si for future FETs



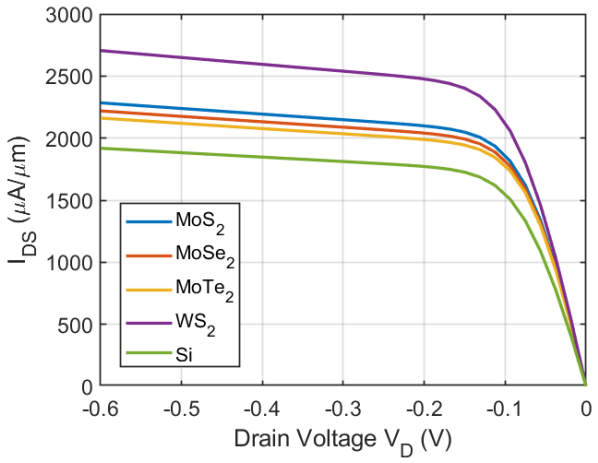


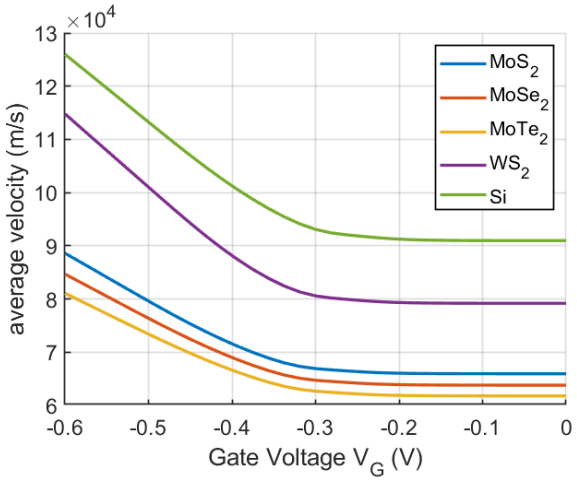
The calculated results of a p-type MOSFET along the k_x direction are presented below. The ON-current of monolayer WS_2 transistors is 1.5 times larger than that of 2-D-Si transistors. Moreover, monolayer MoS_2 transistors outperform 2-D-Si transistors in terms of ON-current by about 27.3%.





Average velocity V_{avg} of carrier at the top of the energy barrier, with increasing gate voltage V_G for p-type monolayer MX_2 and 2-D-Si transistors and IV characteristics are shown:





For a more practical model, the influence of phonon scattering, impurity scattering, and contact resistance should be considered to provide a more complete picture.

It is realized that all of MX2 outperform 2D-Si transistors as well as it is found that the ballistic performances of MoX2 transistors is very similar. WS2 is found to have the best characteristics. They all exhibit better gate controllability because of atomic body thickness thus prove to be very promising devices for future devices.

References:

[1] Liu, L., Kumar, S. B., Ouyang, Y. & Guo, J. Performance limits of monolayer transition metal dichalcogenide transistors. *IEEE Trans. Electron Devices* 58, 3042–3047 (2011)

[2] Rahman, J. Guo, S. Datta, and M. S. Lundstrom, "Theory of ballistic nanotransistors," *IEEE Trans. Electron Devices*, vol. 50, no. 9, pp. 1853–1864, Sep. 2003

[3] S.Datta, Nanoscale Device Modeling: the Green's Function Method, *Superlattices and Microstructures*, vol.28, p.253 (2000)