Insight on the Characterization of MoS₂ Based Devices and Requirements for Logic Device Integration

César J. Lockhart de la Rosa,^{a,b,*,z} Goutham Arutchelvan,^{b,=} Iuliana Radu,^a Dennis Lin,^a Cedric Huyghebaert,^a Marc Heyns,^{a,b} and Stefan De Gendt^{a,c,*}

^aimec, B-3001 Leuven, Belgium

^bKU Leuven, Department of Metallurgy and Materials Engineering, B-3001 Leuven, Belgium

^cKU Leuven, Department of Chemistry, B-3001 Leuven, Belgium

MoS₂ based transistors are being explored as a promising candidate for different applications. The techniques employed to characterize these devices have been directly adapted from 3D semiconductors, without considering the validity of the assumptions. In this work, we discuss the limitations of two-probe (2P), four probe (4P) and transfer length methods (TLM) for extracting electrical parameters. Based on finite-element modeling, we provide design considerations for 4P structures to measure more accurately. Extracting the parameters from these techniques in the appropriate regimes, we identify contact resistance R_C to be critical for scaled MoS₂ devices. Using 4P and TLM measurements along with temperature dependent measurements, we derive further insights into the behavior of the R_C in the subthreshold and linear regime. Additionally, we propose an empirical model for the on-state contact resistance.

© The Author(s) 2016. Published by ECS. This is an open access article distributed under the terms of the Creative Commons Attribution 4.0 License (CC BY, <http://creativecommons.org/licenses/by/4.0/>), which permits unrestricted reuse of the work in any medium, provided the original work is properly cited. [DOI: 10.1149/2.0131611jss] All rights reserved.

Manuscript submitted July 6, 2016; revised manuscript received July 27, 2016. Published August 18, 2016. *This paper is part of the JSS Focus Issue on Properties, Devices, and Applications Based on 2D Layered Materials.*

The ever-growing demand in semiconductor industry for faster, denser, efficient and robust technology has been driving the need for innovative solutions. Though, scaling was very effective in this regard, in recent years there are growing challenges for the conventional three-dimensional (3D) semiconductors.¹ One limitation is the reduced electrostatic control of the gate over the device channel as the channel length (L_{CH}) get smaller. To overcome this problem multi-gate technologies evolved and FINFET structures has become the *de facto* standard for high performance devices. However, even these devices face problems due to, among other things, the 3D nature of these devices.² Another possible solution is to use 2D planar technologies with ultra-thin body semiconductors to allow for better electrostatic control without losing the two-dimensional (2D) nature of the processing and the device. Nevertheless, this cannot be achieved with conventional 3D semiconductors due to performance degradation on thinning below 100 nm. Breaking the out of plane covalent bonds increases the dangling bonds on the surface, resulting in mobility degradation due to surface scattering of electrons.³

In this context, the family of 2D crystals such as graphene and transition metal dichalcogenides (MX₂) offer an interesting case to investigate as alternate ultra-thin body channels. The layers being weakly bonded to each other only by Van der Waals forces and no out-of-plane covalent bonds, there are less dangling bonds than in case of thinning down 3D semiconductors. This enables better electrostatic control while avoiding degradation of transport properties. Among the 2D material crystals, MX₂ are specially interesting due to their semi-conductive properties.⁴⁻⁶ They have also been predicted to have robust performance for channel lengths down to 15 nm.⁷ Molybdenum disulfide (MoS₂), is commonly used as a representative of the MX₂ family. It has been demonstrated to be an interesting candidate for different applications such as low power logic devices, spintronic, valleytronic and also photo-voltaic devices.⁸⁻¹² It is imperative to evaluate certain parameters of MoS₂ and compare them to the actual requirements of industry. Some of the most relevant parameters are (1) the ratio between the on and the off current ($I_{ON/OFF}$), (2) the parasitic resistance (R_C), (3) the field effect mobility of the carriers (μ_{FE}), and the (5) carrier concentration (n_{2D}).

Several methods have been used to characterize these parameters for MoS₂ devices.^{4,9,13} In this work, we discuss the extraction of

mentioned parameters by using two probe (2P), four probe (4P), and Transmission Line Measurements (TLM), clarifying the underneath assumptions and their effect on the MoS₂ device measurements. Extracting the relevant parameters from the techniques, we identify the potential problems in introducing MoS₂ in the industry. Further, we give some insight into the electron transport between the metal-MoS₂ interface with temperature measurements and characterization of effective thermionic emission barrier. Finally, we conclude with comparisons of the extracted parameters with respect to the present requirements from industry and suggestions for improvement.

Technique Discussion and Parameter Extraction

For the measurements and property extraction MoS₂ back-gated 4P-FETs and TLM structures were built. Sketches, optical images and additional information of the devices can be seen in Figure 1. For the fabrication, mechanically exfoliated MoS₂ flakes were transferred to a highly doped Si covered with 55 nm SiO₂. The thickness of the flakes was assessed by atomic force microscopy (AFM) and they ranged between 3.2 nm and 5.91 nm. In Figure 1b a sample of an AFM height profile is shown. The contacts were fabricated using E-beam lithography and lift-off of 70 nm Au metal. After fabrication, the devices were annealed at 140°C for 2 hr in vacuum. For the 2P characterization the device L1 from the TLM set D was used ($L_{CH} = 400$ nm).

Two probe field effect transistors (2P-FET).—These are the easiest to implement and correspond directly to the final transistor to be used. The two probes refer to the source and drain contacts which act as both voltage and current probes. A potential difference (V_{DS}) is applied across these probes and the circulating current (I_{DS}) is measured. I_{DS} is modulated with the gate potential with respect to the source (V_{GS}) by changing the induced carrier concentration in the MoS₂ film. The resulting transfer curve (I_{DS} vs. V_{GS}) can be seen Fig. 2a. The upper axis of the graph is the displacement field ($D = \epsilon_r \times V_{GS}/T_{OX}$). This allows for comparison of the transfer curve with a different gate stack. In this device the total resistance is given by,

$$R_{T(V_{GS})} = R_{P(V_{GS})} + R_{CH(V_{GS})} \quad [1]$$

Where R_{CH} is the channel resistance and the parasitic resistance (R_P) contains all the other undesired resistances as contact resistance (R_C) and the resistance of any un-gated region (R_A) before accessing

*These authors contributed equally to this work.

*Electrochemical Society Fellow.

^zE-mail: lockhart@imec.be

Figure 1. a) Schematic of the 4P measurement setup. b) AFM images, profiles and optical micro-graphs of the device A and tables with dimensions for devices A and B. c) Schematic for the TLM setup. d) Optical micro-graph of device C and table with the dimensions for TLM sets C and D. Device L1 from TLM set D ($L_{\text{CH}} = 400 \text{ nm}$) was used for the 2P analysis.

the gate modulated channel. In case of *low and gate-bias independent* R_P , the threshold voltage (V_{TH}), field mobility and carrier concentration can be obtained from the conventional drain current (I_D) equations for FETs.¹⁴ The square law model provides Equation 2 for linear current $I_{D\text{LIN}}$ and Equation 3 for saturation current $I_{D\text{SAT}}$.

$$I_{D\text{LIN}} = \frac{W_{\text{CH}}}{L_{\text{CH}}} \mu_{\text{FE}} C_{\text{OX}} \left(V_{\text{GS}} - V_{\text{TH}} - \frac{V_{\text{DS}}}{2} \right) V_{\text{DS}} \quad [2]$$

$$I_{D\text{SAT}} = \frac{W_{\text{CH}}}{L_{\text{CH}}} \mu_{\text{FE}} C_{\text{OX}} \frac{(V_{\text{GS}} - V_{\text{TH}})^2}{2} \quad [3]$$

where L_{CH} is the channel length, W_{CH} is the channel width, $C_{\text{OX}} = \epsilon / T_{\text{ox}} = 6.28e - 8 \text{ F/cm}^2$ is the gate stack capacitance for 55 nm SiO_2 and q_e is the electron charge. Thus from these equations it can be seen that the transconductance (Eq. 4) in the linear regime will be constant (Eq. 5) and in the saturation regime it will be linearly depending on $V_{\text{GS}} - V_{\text{TH}}$ (Eq. 6). In Fig. 2b, a plot of the transconductance (gm) obtained from numerical differentiation of I_{DS} can be seen. The plateau in gm, corresponds to the linear operation regime of the FET and mobility is extracted from this peak value using Equation 7. Further, V_{TH} is the V_{GS} value obtained by extrapolating the linear fit of the saturation regime to zero transconductance. The extracted

parameters are listed in Table I.

$$gm = \frac{dI_D}{dV_{\text{GS}}} \quad [4]$$

$$gm_{\text{LIN}} = \frac{W_{\text{CH}}}{L_{\text{CH}}} \mu_{\text{FE}} C_{\text{OX}} V_{\text{DS}} \quad [5]$$

$$gm_{\text{SAT}} = \frac{W_{\text{CH}}}{L_{\text{CH}}} \mu_{\text{FE}} C_{\text{OX}} (V_{\text{GS}} - V_{\text{TH}}) \quad [6]$$

$$\mu_{\text{FE}} = \frac{L_{\text{CH}}}{W_{\text{CH}}} \frac{gm_{\text{LIN}}}{C_{\text{OX}} V_{\text{DS}}} \quad [7]$$

$$n_{2D} = \frac{L_{\text{CH}}}{W_{\text{CH}}} \frac{I_D}{q_e \mu_{\text{FE}} V_{\text{DS}}} = \frac{C_{\text{OX}} V_{\text{GS}} - V_{\text{TH}} - \frac{V_{\text{DS}}}{2}}{q_e} \quad [8]$$

In the case of overlapping back-gated MoS_2 device (as is the case for device D-L1 used in this work and most MX_2 literature), both of the previous assumptions (low R_P and gate independent R_P) for 2P are invalid. First, the value of the parasitic resistance can be considerably higher than in conventional semiconductors and secondly because R_C shows a strong gate-field modulation (demonstrated later with other techniques). This renders the above extraction inaccurate and additional test structures (such as 4P and TLM) are required to de-couple

Figure 2. a) Transfer characteristics for device L1 from TLM set D ($L_{\text{CH}} = 400 \text{ nm}$). b) Transconductance of the same device. Line fitted to determine V_{TH} and peak used to extract peak transconductance and mobility. c) Fitting to total resistance of the device for the regime where transconductance is mostly constant (linear regime). The data clearly fit to the model and the extracted mobility ($22.71 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$) is higher than the original mobility obtained without excluding the effect of R_C ($14.5 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$).

Table I. Extracted electrical characteristics from different techniques.

	A 4P	B 4P	C TLM	D TLM	D-L1 (0.4μm) 2P	D-L1 (0.4μm) 2P-Fitting	Literature ^{9,13}	Units
T _{MoS₂}	3.2	4.6	5.91	3.13	3.13	3.13	[1.4, 2.8]	nm
I _{ON/OFF} (G _{ON/OFF})	6.1E7	2.2E7	(6.5E7)	(1.2E8)	8.3E7	8.3E7	>1E8	-
V _{TH} (V _{TH} average)	-6.6	-13.8	(-8.05)	(-4.75)	-5.75	-5.75	-	V
μ _{FET}	27	26	19	21	15	23	[16, 30]	cm ² V ⁻¹ s ⁻¹
R _{SH} (V _{GS} = V _{TH})	1.85E7	8.3e6	2.6E6	5.22E6	6.99e6	-	-	Ω/□
R _{SH} (V _{GS} = 30 V)	2.2e4	1.9e4	3.2E4	3.6E4	4.13e4	1.9E4	-	Ω/□
n _{2D} (V _{GS} = 0 V)	1.3E12	2.6E12	7.1E11	2.9E11	5.2E11	-	-	cm ⁻²
n _{2D} (V _{GS} = 30 V)	1.1E13	1.3E13	1.1E13	9.5E12	1.0E13	1.3E13	-	cm ⁻²
R _C (min)	2.51 K	3.25 K	3.13 K	2.8K	-	4.4 K	4.7 K	Ω*μm
ρ _C (V _{GS} = 30 V)	-	-	3.1e-6	2.4E-6	-	-	-	Ω*cm ²
L _T (V _{GS} = 30 V)	-	-	101	88	-	-	-	nm

R_{CH} from R_P. However, in this work, we provide an empirical relationship for R_C that would still allow us to reliably extract parameters from 2P measurements and give a good estimation of R_P as a function of V_{GS}. We observe from other measurement techniques and fittings discussed in future sections, that gate-dependent R_C in MoS₂ FETs exhibit a 1/V_{GS} dependency in the linear operation regime to a good approximation as shown in Figure 10a.

Thus the 2P R_T in the linear regime is modeled with Equation 1 and R_P and R_{CH} are fitted as follows,

$$R_P = 2 R_{C(V_{GS})} = \frac{2}{A(V_{GS} - V_{TH}) + B} \quad [9]$$

$$R_{CH(V_{GS})} = \frac{L_{CH}}{W_{CH} \mu_{FET} C_{OX} (V_{GS} - V_{TH})} \quad [10]$$

For the case of overlapping gates as the whole channel is gated the access resistance (R_A) can be considered zero, and thus the R_C is the main contributor to R_P (Eq. 9). From the observations on the behavior of R_C extracted in the next section R_C can be empirically expressed as Equation 9. R_{CH} is obtained from Equation 2 for the case when the absolute value of |V_{GS}-V_{TH}| ≫ |V_{DS}/2|. The intrinsic mobility (without the effect of R_C) and the pre-factor of R_C are obtained by least-square fitting to the 2P experimental data. V_{TH} is still extracted by the methodology suggested above because the position for the onset of accumulation is not expected to be drastically affected by R_C. Figure 2c shows that the aforementioned fitting method provides a good fit to the data. The extracted parameters are shown in Table I. The mobility obtained from the fit is higher compared to previous extraction without the R_C correction indicating that neglecting R_C could lead to underestimation of the field mobility, specially for scaled devices where the R_{CH} is in the same order of R_C. Additionally, the fitting also allows to evaluate R_C (4.4K ohm @VGS = 30V) for different gate bias without the need to build complicated test structures. Note that for back-gated devices, assuming constant R_C in Equation 1 it yields poor fit with unrealistic values for both the mobility and contact resistance.

Four probe field effect transistors measurements (4P-FET).—

Unlike 2P, provide a direct way to measure R_{CH} and extract mobility without the effect of contact resistance. It also provides an advantage over TLM (discussed later) for contact resistance determination, by allowing to examine source and drain resistances independently. The measurement setup is similar to 2P configuration except that the channel potential is now sensed with two additional probes P1 (V_{P1}) and P2 (V_{P2}) as shown in Figure 1a. By doing some the channel potential can be directly measured excluding the effects of R_C. No potential drop is assumed in the contact between probes P1 and P2 due to the low current drawn by the high impedance voltmeter (>1E + 12 ohm) connected to them.

For a constant V_{DS} ≪ (V_{GS}-V_{TH}), I_{DS} is modulated by varying V_{GS} and the channel potentials (V_{P1} and V_{P2}) are measured for each V_{GS}. The sheet resistance and field mobility can then be extracted

using Equations 12 and 14 respectively from the extracted channel potential (Eq. 11).

$$V_{CH} = V_{P2} - V_{P1} \quad [11]$$

$$R_{SH} = \frac{W_{CH}}{L_{4P}} \times \frac{V_{CH}}{I_D} \quad [12]$$

$$G_{SH} = \frac{1}{R_{SH}} \quad [13]$$

$$\mu_{FE} = \frac{dG_{SH}}{dV_{GS}} \times \frac{1}{C_{OX}} \quad [14]$$

$$n_{2D} = \frac{G_{SH}}{q_e \mu_{FE}} \quad [15]$$

As V_{DS} ≪ V_{GS}-V_{TH}, the accumulation layer can be considered to be uniform along the channel and hence the sheet resistance should also be uniform throughout. Then, by linear extrapolation the contact resistances at the source (R_{CS}) and drain (R_{CD}) are determined independently from the measured potentials in P1 and P2 respectively as shown in Equations 16 and 17.

$$R_{CS} = \frac{V_{P1} - V_{SS}}{I_D} - \frac{L_{SP1}}{W_{CH}} \times R_{SH} \quad [16]$$

$$R_{CD} = \frac{V_{DS} - V_{P2}}{I_D} - \frac{L_{DP2}}{W_{CH}} \times R_{SH} \quad [17]$$

where L_{SP1} and L_{DP2} are the distances from the source and drain contacts to the center of P1 and P2 probes, respectively. Nevertheless, the accuracy of the measured potentials and subsequent extrapolations depend sensitively on the device geometry. This is mainly because the 4P approach relies on the assumption that the introduction of voltage probes does not alter the potential distribution of the FET and this consideration will not hold for all geometries.

In order to investigate the effect of geometry on the measurements, a 2D finite-element model was created to study the changes of the channel potential in the linear regime for different potential probe configurations. The design investigated has source and drain contacts placed at the edge of a rectangular flake. Source and drain contacts were treated as ohmic and conductivity of the channel was assumed to be spatially uniform and varying only with gate-bias. The probes P1 and P2 of equal lengths (L_P) are centered at one-third and two-thirds of the channel length (L_{CH} = 2.5 μm) respectively. Three different L_P (100 nm, 300 nm and 500 nm) were simulated with 6 different levels of intrusion into the channel from non-invasive (Y = 0 μm) to completely invasive (Y = 1.4 μm) to understand the potential profile perturbation.

Figure 3a shows the simulated equipotential lines in the device under bias conditions V_{DS} = 1 V and V_{GS} = 30 V for L_P = 300 nm (L_P ≈ L_{CH}/10) with an intrusion length of 100 nm from the flake edge. The equipotential lines are slightly altered around P1 and P2 as marked (Fig. 4a). As the probes intrude into the channel, electrons

Figure 3. a) Simulated potential contour in a 4P-FET. b) Effect of probe length geometry in the extracted value of R_{SH} . As it can be seen ideally the probe should intrude as minimum as possible into the channel of the device.

can flow from the source to the drain through the parallel path of the metal probes P1 and P2 if this resistance is less than that through the channel. This will cause an increase of the total current and further uncertainty with respect to the measured V_{P1} and V_{P2} . As a result the calculated sheet resistance using Equation 12 can be underestimated as shown in Fig. 3b. This difference in sheet resistance can also lead to overestimation of contact resistance when extrapolated to the contacts (from Equations 16 or 17). From the model it can be inferred that ideally voltage probes with length ten-times smaller than the channel length and with minimum intrusion are preferable for more accurate measurements.

In MoS₂ 4P devices, in order to avoid a shaping step in the fabrication process, P1 and P2 are positioned in the perimeter of the naturally shaped flake. The previously mentioned considerations are taken into account. In our experiments, the probe intrusion are about 300 nm for device A and 280 nm for device B. Given the fact that the channel widths of the devices are 3.1 μm and 2.5 μm for A and B respectively, the aforementioned probe intrusions are comparable to an intrusion of about 100 nm in Figure 3a ($W_{CH} = 1 \mu m$). Further, the length of the probes is 300 nm, for $L_{CH} = 2.5 \mu m$. Thus, the underestimation of R_{SH} for our devices are represented by the green dot on the red-line of Figure 3b. An error of 3.9% is then expected for the values extracted from these devices. In Figure 4, results of the 4P measurements for the device A can be seen and the extracted parameters are listed in Table I. The mobility of $26.75 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ is higher than the mobility extracted from the 2P device without excluding R_C ($14.5 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$), but similar to the mobility extracted using Equation 9 to fit and exclude the effect of R_C in the same 2P measurement ($22.71 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$). This demonstrates that the empirical

model is a good option to gain some understanding while using 2P devices. The threshold voltage is extracted similar to the 2P technique using Equation 6. Additionally the source contact resistance (R_{CS}) and drain contact resistance (R_{CD}) were extracted as shown in Figure 4c. We observe that for $V_{GS} > V_{TH}$ the source and drain resistances are similar in magnitude and exhibit identical gate-field dependency.

Transmission line measurements (TLM).—These allows to evaluate sheet resistance, contact resistance and additionally contact resistivity and transfer length from a set of 2-P devices with varying channel-length adjacent to one another. A representative sketch of the setup and optical image of the device can be seen in Figure 1c and Figure 1d. The voltage and current are sensed across the same contacts similar to 2P. In TLM, the contact region is modeled as a resistor ladder as shown in the inset of Figure 5a and when current flows from semiconductor to the metal it naturally chooses the path of least resistance. The potential drop along the contact according to^{15,16} is given as,

$$V(x) = \frac{I\sqrt{R_{SH}\rho_c}}{W} \frac{\cosh[(L_C - x)/L_T]}{\sinh(L_C/L_T)} \quad [18]$$

$$L_T = \sqrt{\rho_c/R_{SH}} \quad [19]$$

where I is the current through the contact, R_{SH} is the sheet resistance of the semiconductor under the contact, ρ_c is the specific contact resistivity, L_C is the contact length and L_T is the characteristic injection length or transfer length. L_T is considered as the distance over which significant current injection happens under the contact. This phenomenon is generally termed as *current crowding*. From

Figure 4. a) Potentials in S, P1, P2 and D contacts as a function of V_{GS} . It can be seen that the potential drop is linear across the device. b) Sheet conductance extracted from the 4P device where the effect of the contact resistance is excluded. The extracted mobility is ($26.75 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$) is similar to the one extracted from the fitted 2P device ($22.71 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$). R_C extracted from 4P setup for the source contact, the drain contact and the average of both. It is clearly seen that R_{CS} and R_{CD} are very similar for the case when $(V_{GS} - V_{TH})$ is bigger than V_D .

Figure 5. a) Evaluation of the hyperbolic cotangent for different contact lengths. In this experiments $L_C = 300 \text{ nm}$, thus it can be safely assume that $\coth(L_C/L_T) \approx 1$. In the insight, the resistor network model of the metal/semiconductor interface. b) Example of parameters extraction from TLM for device D at $V_{GS} - V_{TH} = 31.8 \text{ V}$. The yellow square intersecting R_T axis represents $2R_C$ and the intersection of the L_{CH} axis represents $2L_T$. The slope of the line is used to extract R_{SH} .

Equation 18, the contact front resistance at $x = 0$ (Figure 5a) is given as,

$$R_C = \frac{V}{I} = \frac{\sqrt{R_{SH}\rho_c}}{W} \coth(L_C/L_T) \quad [20]$$

$$R_C = \frac{R_{SH} L_T}{W} \coth(L_C/L_T) \quad [21]$$

With the approximation $L_C > 1.5 L_T$ (Figure 5a), Equation 21 reduces to,

$$R_C = \frac{R_{SH} L_T}{W} \quad [22]$$

From above equation, the total resistance (R_T) for each 2P device is given as,

$$R_T = 2R_C + R_{SH} \left(\frac{L_{CH}}{W_{CH}} \right) = \frac{R_{SH}}{W_{CH}} (2L_T + L_{CH}) \quad [23]$$

Note the final expression above assumes linear regime operation.

For our experiments, we fabricated two sets of TLM structure each with three different channel lengths. Each TLM set is built on a single flake to ensure minimum variability between the contacts of individual devices in the set. Details of device dimensions are provided in Figure 1d. Transfer curve for the TLM set D is shown in Figure 6a. Generally, a slight threshold shift is observed between the devices of a TLM set and this is corrected by aligning to a common V_{TH} before using Equation 23 to evaluate the resistances for the same gate overdrive voltage across the devices. Plotting R_T Vs L_{CH} , as the method suggests, the sheet resistance, contact resistance and transfer length (and hence contact resistivity from Equation 24) can be obtained from the slope, R_T intercept and L_{CH} intercept, respectively, for each V_{GS} . An example is shown in Figure 5b.

$$\rho_c = R_C L_T W_{CH} \quad [24]$$

Mobility is extracted from the sheet resistance (Figure 6b) using Equations 13 and 14 and the value ($\approx 21 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$) is in good agreement with those obtained from previous techniques. We observe a strong gate modulated R_C with magnitudes similar to the 4P measurement (Figure 6c). The current crowding model provides further insights on R_C modulation. As Equation 22 demonstrates, even a constant transfer length would exhibit a gate-modulated R_C as charge is injected in MoS_2 film changing R_{SH} . This dependence on R_{SH} gives rise to the $1/V_{GS}$ modulation for the contact resistance. Figure 6d shows that the transfer length is not constant during the whole regime but arrive to a plateau where it is rather constant. As a result, the

extracted contact resistivity using Equation 24 (ρ_c) is also changing as $1/V_{GS}$ (Figure 6e). The lowest contact resistivity for our device is about $2.4 \times 10^{-6} \text{ Ohm} \times \text{cm}^2$.

Additionally, the contact resistance is compared to the channel resistance of devices with L_{CH} equal to 100 nm , 200 nm , 400 nm and 2500 nm . The result can be seen in Figure 6f. It is clear that for L_{CH} smaller than 100 nm the contact resistance will be equal or even higher than the channel resistance, making R_C the dominant resistance of the device. Therefore, scaling L_{CH} below 100 nm requires that the problem of high R_C and ρ_c be addressed.

For more insights on R_C and ρ_c we have conducted temperature dependence studies to identify any thermally activated mechanism.

Thermionic emission in the the Metal/ MoS_2 interface.—Schottky Barrier is formed between MX_2 and the metal due to the work function difference between the two materials. Unlike conventional semiconductor, the ultra-thin body of MX_2 makes it difficult for doping via traditional methods and in the subthreshold regime where the accumulation layer under the contact is not completely formed, the barrier width could be significant. Hence transport mechanisms such as thermionic emission and direct or Fowler-Nordheim tunneling (Figure 8b) could determine the contact resistivity.

Figure 8a, shows the band-diagram of MX_2 FET in the subthreshold regime. Two Schottky diodes are connected back to back with the channel in between. For a potential difference of $V_{DS} > 3 \text{ KT}/q$ and $V_{GS} < V_{TH}$, the drain-diode is forward-biased and source-diode is reverse-biased. With increasing gate bias, the V_{DS} is predominantly dropped at the largest of three sources of resistance - source junction, drain junction or the channel. If the Schottky barrier is presumed to limit the current, then the reverse-biased junction at the source will dominate. Then, 3D-thermionic emission Equation 25, where the barrier ϕ_{SB} is replaced by an effective barrier ϕ_{eff} is used to model the current across the source junction and access the barrier modulation with V_{GS} .¹⁷

$$I = A A^{**} T^2 \exp\left(\frac{-q_e \phi_{eff}}{K_B T}\right) \exp\left(\left(1 - \frac{1}{n}\right)\left(\frac{q_e V_{\Delta S}}{K_B T}\right)\right) \quad [25]$$

$$V_{\Delta S} \approx -V_{DS} \quad [26]$$

In this equation A is the area where current is flowing, A^{**} is the Richardson constant, T is the temperature in K, n is the ideality factor and K_B is the Boltzmann constant.

Experimentally, a set of transfer curves I_D - V_{GS} for different V_{DS} is measured for a range of temperatures (typically between 270 K

Figure 6. Extracted values from TLM device set D. a) Transfer characteristics for independent devices. The I_{ON} current increased from 68 $\mu\text{A}/\mu\text{m}$ to 136 $\mu\text{A}/\mu\text{m}$ for L_{CH} equal to 400 nm and 100 nm respectively. The factor of 2 increase is clearly not following the expected factor of 4 decrease in L_{CH} . Extracted R_{CH} (b), R_C (c), L_T (d) and ρ_C (e) of the TLM set D. The blue background indicate the error margin from the TLM fitting. f) Comparison of different channel resistances with respect to the extracted contact resistance. For L_{CH} equal or smaller than 100 nm R_C start to dominate total resistance, thus before reducing L_{CH} below 100 nm the high values of R_C need to be addressed.

and 350 K). From these set of measurements, Arrhenius plot (Equation 27) is derived as shown in Figure 9a for each V_{GS} and from the slope of the Arrhenius plot, effective barrier ϕ_{eff} can be obtained by extrapolating the value of S (Equation 28 and Figure 9b) to $V_{DS} = 0$ V. Thus, the barrier modulation with V_{GS} is obtained as in

Figure 9c.

$$\ln\left(\frac{I}{T^2}\right) = C + \left(\frac{q_e}{K_B T}\right) \left(-\phi_{eff(V_{GS})} + V_{DS} \left(-1 + \frac{1}{n}\right)\right) \quad [27]$$

Figure 7. a) Fitting to R_C extracted from TLM to demonstrate the behavior of R_C modelled in Equation 9. b) Comparison of the contact resistance as obtained from TLM structures, 4P devices and 2P fitting. The minimum values for each method was 2.8 K $\Omega \mu m$, 2.5 K $\Omega \mu m$ and 4.4 K $\Omega \mu m$ respectively. It can be clearly seen that the values extracted from 4P and TLM are very similar specially for the regions of V_{GS} where the transconductance of the device remain constant. The extracted R_C from fitting is about a factor of 1.6 higher than the extracted R_C from TLM and 4P, nevertheless is a good estimation considering the simplicity of the setup. This fitting technique is suited to give a good estimation when working with scaled 2P devices.

$$S(V_{DS}, V_{GS}) = -\phi_{eff}(V_{GS}) + V_{DS} \left(-1 + \frac{1}{n} \right) \quad [28]$$

$$\phi_{eff}(V_{GS}) = -S(0, V_{GS}) \quad [29]$$

The effective barrier decreases monotonically with increase in V_{GS} but with two different slopes approximately around $V_{GS} = V_{FB}$. Furthermore, the effective barrier is reduced to 0 eV around V_{TH} and this can also be noticed in the change of temperature coefficient for the total resistance ($I_D - V_D$). For $V_{GS} < V_{FB}$, a positive temperature coefficient (conductivity decreases with decrease in temperature) is

noticed, characteristic of thermionic emission over the barrier (Figure 8e). For $V_{GS} > V_{TH}$, the barrier width is thin enough (indicated by 0 eV) and tunneling mechanisms could dominate at the contacts leading to the total resistance limited by the heavily doped channel, suggested by the negative temperature coefficient (conductivity increase with decrease in temperature- Figure 8f). Thus, the intrinsic barrier height can be defined as the value of ϕ_{eff} at the point when it deviates from its linear dependence with V_{GS} . This point also defines the flatband state of the device. The flatband barrier height for different elemental metals to MoS_2 is reported in Table II. We noticed that the extracted barrier heights differ significantly from the

Figure 8. a) Band diagram of the device when a positive V_{DS} is applied and equivalent electronic circuit. b) Transport mechanisms taking place in the Metal/ MoS_2 interface. c) Band diagram of the parameters and model being considered for the extraction of the effective SB. d) Surface plot of the measured current as a function of V_{GS} and V_{DS} for a MoS_2 -FET with Au contacts at room temperature. e) Output characteristics of the device as a function of temperature in the subthreshold regime ($V_{GS} = -13$ V. f) Output characteristics of the device as a function of temperature in the lineal regime ($V_{GS} = 14$ V. The change in the trend of the current with temperature demonstrate that thermionic emission is not the dominant mechanism when charge has been accumulated in the MoS_2 layer.

Table II. Extracted Φ_{SB} and ideal Φ_{SB} by considering only the difference in work function and electron affinity.

	Measured	Ideal	Literature
Ni/MoS ₂	248 meV	~600 meV	100 meV ¹³
Mo/MoS ₂	93 meV	~100 meV	-
Au/MoS ₂	340 meV	~600 meV	45 meV ⁹

theoretical values obtained from the difference between metal work function and MoS₂ electron affinity. This discrepancy can be explained by the fermi level pinning due to metal induced gap states in the MoS₂ film interface as previously reported for conventional semiconductors.¹⁸

General observations of characterization techniques.—Consistently across the different measurement techniques, we note that the contact resistance is significantly modulated by gate overlap with the contacts. In the subthreshold regime, this gate dependency could be predominantly due to the modulation of ϕ_{SB} by the gate bias and subsequent thinning of Schottky barriers at the source and drain contacts for V_{GS} above flatband potential. This is substantiated by the change from positive to negative temperature coefficient of the total conductivity and the low or negative ϕ_{eff} as the gate is swept from subthreshold to accumulation regime. This was observed independently of the nature of the metal used.

In the linear regime, the accumulation layer has sufficiently thinned down the barrier and the R_C seems to depend only in the reduction of R_{SH} , as explained by the current crowding model. The model also points out that contact resistivity is significantly modulated by V_{GS} . The 4P analysis corroborates the observation on the transparency of Schottky barrier in the linear regime and shows that both the carrier injection (at source contact) and carrier extraction (at drain contact) exhibit similar resistance (within experimental errors) hinting at injection mechanism different from subthreshold region. Additionally, we use the values of R_C extracted from TLM set D and demonstrate that it fits to the model we state in Equation 9 to fit the total resistance and extract the parameters of a 2P devices excluding contact resistance (Figure 7a). Also, the values of the contact resistance from all the methods we have used in order to compare were plotted and shown in Figure 7b. The values extracted from 4P and TLM are very similar as expected. However for the case of the value from 2P device fitting we see that there is an overestimation of R_C with respect to the other techniques. Nevertheless, considering that a 2P device was used and that the device was 400 nm it is clearly an interesting option. From the above analysis, it is evident that R_C and ρ_C plays a significant role in the integration of MX₂ devices.

Figure 10. Schematic with the dimensions of the ideal MoS₂ device according to the industry requirements for 2019 in the high performance core logic group.

Technology Requirements

Following the projections of the International Technology Roadmap for Semiconductors (ITRS 2.0) the earliest that TMDC can be introduced to industry would be the period 2018-2023.¹⁹ At 2019 the required half pitch (channel length) for high performing devices will be of 21 nm (14 nm) for high performance devices. That will signify a contact area of only about 14 nm. These dimensions are sketched in Figure 10. Considering the electron mean free path of a perfect MoS₂ layer is about 15 nm²⁰ it is possible that mobility will not be our main concern. Even if in real devices due to natural defect this were not the case and the mean free path were smaller, the biggest problem will still be the R_C . Not only because as the L_{CH} is much smaller than the 100 nm specified in previous sections but also because the contact length (L_C) is smaller than the transfer length determined from TLM (Figure 6d). This will mean that we actually would be in the red region of Figure 5a and thus the actual approximation for $\coth(L_C/L_T)$ in Equation 21 will be $1/L_C$ instead of 1 and thus instead of Equation 22 the approximation for R_C will be:

$$R_C = \frac{R_{SH} L_T}{W L_C} \quad [30]$$

And thus the contact resistance will increase by a factor of $1/L_C$ with respect to the case where the contact was longer than the transfer length worsening even more the performance of the device for the specific case of 13 nm the measured contact resistance will increase from $2.8 \text{ K}\Omega \times \mu\text{m}$ to about $280 \text{ K}\Omega \times \mu\text{m}$ while the channel resistance that at 100 nm was already very similar to the contact resistance (Figure 6f) will decrease by a factor of 7. This will make the R_C of the device almost 3 order of magnitude higher than the channel resistance. As it can be seen from Figure 11 several attempts

Figure 9. a) Arrhenius plot obtained from Equation 27. b) S parameter as a function of V_{DS} (Equation 28). c) Effective ϕ_{SB} extracted as a function of V_{GS} . The reported value for Au contact (340 meV) is taken from the flatband region of the device, when the linear dependence of ϕ_{SB} with respect to V_{GS} is lost.

Figure 11. Different contact resistance reported in literature for optimization through Metal/MoS₂ interface engineering and through doping.^{13,21–25}

has been done to reduce the contact resistance.^{13,21–25} These trials can be divided in two main fields: engineering the interface and doping the MoS₂ film. For engineering the interface, different metals has been used with Ni, Au, and Mo being the most popular choice and Mo and Au presenting the lowest R_C . Other way of engineering the interface is by introducing a material in between the metal and the 2D material. The most successful strategy in this field was by introducing graphene layers in between. Furthermore, the lowest r_C ($200 \text{ ohm} \times \mu\text{m}$) correspond to the case where one additional layer of patterned graphene is introduced in addition to the normal graphene layer.²¹ The second strategy is to dope the MoS₂ film to reduce the sheet resistance. By doing so the R_C has been reduced down to about $500 \text{ ohm} \times \mu\text{m}$ for the case of chloride doping.²² Further decrease of R_C could be achieved by combining both strategies. Nevertheless, even for the lowest reported R_C to our knowledge ($200 \text{ ohm} \times \mu\text{m}$)²¹ the R_C will be at least 2 order of magnitude higher than the channel resistance for the required dimensions.

Also from Figure 6c it can be seen that even for high V_{GS} when thermionic emission is not expected to dominate the transport from the contact to the MoS₂ film the contact resistivity still remains very high ($2.4\text{E-}6 \text{ Ohm} \times \text{cm}^2$) far from the ideal value of $1\text{E-}9 \text{ Ohm} \times \text{cm}^2$ desired in technology. A possible explanation could be a large direct tunneling barrier that the electrodes need to overcome or a fully depleted region under the contact limiting carrier injection. Nevertheless further research is required to reduce its value.

Conclusions

In summary, we have compared the validity of different electrical test structures in evaluating parameters such as field mobility, threshold voltage, contact resistance and contact resistivity. We have provided corrections such as gate bias-dependent empirical model for R_C in case of 2P and recommendation for device geometries for 4P and TLM to reliably extract the above mentioned parameters for MoS₂ FETs. Particularly, we have modeled 4P setup and evaluated its accuracy for invasive and long voltage probes. The design considerations were further used in our experiments to evaluate the behavior of source and drain resistances independently in the linear regime. These results were in agreement with those from TLM structures and the following conclusions can be draw:

In the linear regime, field effect mobility can be reliably extracted from the plateau in the gm curve for long channel devices. For short-channel devices, the contact resistance is comparable or equal to the channel resistance and either 4p or TLM would be required to decouple R_{CH} from R_C . The contact resistance at source and drain are similar in magnitude and exhibit $1/V_{GS}$ dependency. From the current crowding model, we can infer that improving sheet resistance can lead to a reduced contact resistance. Also, the contact resistivity

exhibits a strong gate dependency and the underlying physics needs to be understood. In the subthreshold regime, temperature dependence measurement yield an effective barrier for the devices which can be reduced with increased gate-field. Finally we compare the extracted parameters with the technology requirements following the industry requirements and identified the contact resistivity and thus the parasitic contact resistance as the major challenges that need to be addressed before scaling the devices below 100 nm .

Acknowledgment

The authors thank the laboratory personnel, J. Loo, K. Baumanns, and J. De Cooman for their excellent technical work. Also they thanks for financial support to the Beyond CMOS program at imec and to the Research Foundation-Flanders, Belgium (FWO).

References

- N. Z. Haron and S. Hamdioui, "Why is CMOS scaling coming to an END?" *2008 3rd International Design and Test Workshop*. 2008, pp 98–103.
- M. Jurczak, N. Collaert, A. Veloso, T. Hoffmann, and S. Biesemans, "Review of FINFET technology", *SOI Conference, 2009 IEEE International*. 2009, pp 1–4.
- A. Alian, M. A. Pourghaderi, Y. Mols, M. Cantoro, T. Ivanov, N. Collaert, and A. Thean, "Impact of the channel thickness on the performance of ultrathin InGaAs channel MOSFET devices", *2013 IEEE International Electron Devices Meeting*. 2013, pp 16.6.1–16.6.4.
- B. Radisavljevic, A. Radenovic, J. Brivio, V. Giacometti, and A. Kis, "Single layer MoS₂ transistors", *Nature Nanotechnology*, **6**, 147 (2011).
- A. Splendiani, L. Sun, Y. Zhang, T. Li, J. Kim, C.-Y. Chim, G. Galli, and F. Wang, "Emerging photoluminescence in monolayer MoS₂", *Nano Letters*, **10**, 1271 (2010).
- S. Kim, A. Konar, W.-S. Hwang, J. H. Lee, J. Lee, J. Yang, C. Jung, H. Kim, J.-B. Yoo, J.-Y. Choi et al., "High-mobility and low-power thin-film transistors based on multilayer MoS₂ crystals", *Nature Communications*, **3**, 1011 (2012).
- Y. Yoon, K. Ganapathi, and S. Salahuddin, "How good can monolayer MoS₂ transistors be?", *Nano Letters*, **11**, 3768 (2011).
- H. Wang, L. Yu, Y.-H. Lee, Y. Shi, A. Hsu, M. L. Chin, L.-J. Li, M. Dubey, J. Kong, and T. Palacios, "Integrated circuits based on bilayer MoS₂ transistors", *Nano Letters*, **12**, 4674 (2012).
- B. Radisavljevic and A. Kis, "Mobility engineering and a metal-insulator transition in monolayer MoS₂", *Nature Materials*, **12**, 815 (2013).
- D. Xiao, G.-B. Liu, W. Feng, X. Xu, and W. Yao, "Coupled spin, and valley physics in monolayers of MoS₂ and other group-VI dichalcogenides", *Physical Review Letters*, **108**, 196802 (2012).
- H. Zeng, J. Dai, W. Yao, D. Xiao, and X. Cui, "Valley polarization in MoS₂ monolayers by optical pumping", *Nature Nanotechnology*, **7**, 490 (2012).
- S. Wi, H. Kim, M. Chen, H. Nam, L. J. Guo, E. Meyhofer, and X. Liang, "Enhancement of photovoltaic response in multilayer MoS₂ induced by plasma doping", *ACS Nano*, **8**, 5270 (2014).
- H. Liu, A. T. Neal, and P. D. Ye, "Channel length scaling of MoS₂ MOSFETs", *ACS Nano*, **6**, 8563 (2012).
- S. M. Sze and K. K. Ng, *Physics of semiconductor devices*, John Wiley & Sons, Inc. (2007).
- H. H. Berger, "Contact resistance and contact resistivity", *J. Electrochem. Soc.*, **119**, 507 (1972).

16. H. H. Berger, "Models for contacts to planar devices", *Solid-State Electronics*, **15**, 145 (1972).
17. E. H. Rhoderick, "Metal-semiconductor contacts", *IEE Proc.*, **129**, 1 (1982).
18. R. T. Tung, "The physics and chemistry of the Schottky barrier height", *Appl. Phys. Rev.*, **1**, 011304 (2014).
19. Table: Emerging research materials, alternate channel materials.
20. K. Kaasbjerg, K. S. Thygesen, and K. W. Jacobsen, "Phonon-limited mobility in n-type single layer MoS₂ from first principles", *Physical Review B*, **85**, 115317 (2012).
21. W. S. Leong, X. Luo, Y. Li, K. H. Khoo, S. Y. Quek, and J. T. L. Thong, "Low resistance metal contacts to MoS₂ devices with nickel-etched-graphene electrodes", *ACS Nano*, **9**, 869 (2015).
22. L. Yang, K. Majumdar, H. Liu, Y. Du, H. Wu, M. Hatzistergos, R. Tieckelmann, W. Tsai, C. Hobbs, and P. D. Ye, "Chloride molecular doping technique on 2D materials: WS₂, MoS₂", *Nano Lett.*, **14**, 6275 (2014).
23. J. Kang, W. Liu, and K. Banerjee, "High-performance MoS₂ transistors with low-resistance molybdenum contacts", *Appl. Phys. Lett.*, **104**, 093106 (2014).
24. D. Kiriya, M. Tosun, P. Zhao, J. S. Kang, and A. Javey, "Air-stable surface charge transfer doping of MoS₂ by benzyl viologen", *Journal of the American Chemical Society*, **136**, 7853 (2014).
25. Y. Du, H. Liu, A. T. Neal, M. Si, and P. D. Ye, "Molecular doping of multilayer MoS₂ field-effect transistors: Reduction in sheet and contact resistances", *IEEE Electron Device Letters*, **34**, 1328 (2013).