Combined electrical transport and capacitance spectroscopy of a MoS₂ – LiNbO₃ field effect transistor

Władysław Michaiłow,¹, a) Florian J. R. Schülein,¹, ² Benjamin Möller,¹ Edwin Preciado,³ Ariana E. Nguyen,³ Gretel Von Son,³ John Mann,⁴ Andreas L. Hörrner,¹ Achim Wixforth,¹, ² Ludwig Bartels,³ and Hubert J. Krenner¹, ², b)

¹) Lehrstuhl für Experimentalphysik 1 and Augsburg Centre for Innovative Technologies (ACIT), Universität Augsburg, Universitätsstr. 1, 86159 Augsburg, Germany
²) Nanosystems Initiative Munich (NIM), Schellingstr. 4, 80799 München, Germany
³) Chemistry, Materials Science & Engineering and Electrical Engineering, University of California, Riverside, California 92521, United States
⁴) Department of Physics, Pepperdine University, Malibu, California 90263, United States

We have measured both the current-voltage (I_SD-V_GS) and capacitance-voltage (C-V_GS) characteristics of a MoS₂ – LiNbO₃ field effect transistor. From the measured capacitance we calculate the electron surface density and show that its gate voltage dependence follows the theoretical prediction resulting from the two-dimensional free electron model. This model allows us to fit the measured I_SD-V_GS characteristics over the entire range of V_GS. Combining this experimental result with the measured current-voltage characteristics, we determine the field effect mobility as a function of gate voltage. We show that for our device this improved combined approach yields significantly smaller values (more than a factor of 4) of the electron mobility than the conventional analysis of the current-voltage characteristics only.

After the rise of graphene¹–³, a wide range of two-dimensional (2D) materials⁴ shifted into focus of fundamental and applied research⁵. One particularly important class of 2D materials are transition metal dichalcogenides (TMDs)⁶. One important representative TMD is molybdenum disulfide, MoS₂, whose indirect band gap changes to a direct one when its thickness is reduced to one single monolayer⁷–⁹. The resulting high optical activity and sizable bandgap of ~ 1.9 eV make this material ideally suited for optoelectronic applications⁹ and, thus the optical and electronic properties of MoS₂ and related materials have been investigated intensively in the last years¹⁰. In particular, field effect transistors (FETs) and logical circuit prototypes have been devised and realized¹¹–¹³. In such devices, source and drain contacts are patterned onto the TMD film, and the charge carrier density is controlled by gate contacts. For FET devices, the transport mobility of the charge carriers in the conducting channel is of paramount importance. Here, different approaches exist to derive this key figure for FET devices. The most commonly applied method is to measure the source-drain current I_SD as a function of the gate voltage V_GS. Then, the field effect mobility μ_FE is determined from a tangent to the linear region of the I_SD(V_GS)-dependence using the following formula known from FET theory:

$$\mu_{FE} = \frac{\partial I_{SD}}{\partial V_{GS}} \frac{A}{C(V_{GS})} \frac{L}{w} \frac{1}{V_{SD}}.$$ (1)

Here, C(V_GS)/A is the capacitance per unit area, V_SD the source-drain voltage, \(\frac{\partial I_{SD}}{\partial V_{GS}}\) the slope of the linear region, L the length and w the width of the conducting channel. The intersection of the tangent with the abscissa represents the threshold voltage, V_TH. However, this simple FET formula (1) assumes that the mobility is independent of the gate voltage. Moreover, the underlying parallel-plate capacitor model used to quantify the capacitance¹⁴ assumes perfectly conducting, infinitely large plates. These assumptions may represent an oversimplification for 2D semiconductors¹⁵,¹⁶. To quantify the capacitance more precisely, Radisavljevic and coworkers¹⁷ followed an indirect approach: the capacitance was determined from the carrier density obtained from Hall effect measurements and used in equation (1). This helps getting more reliable capacitance values than the ones from the parallel-plate capacitor formula, but the gate voltage dependence was not investigated.

In this Letter, we present an easy to implement approach to determine the carrier density and carrier mobility of a MoS₂ – LiNbO₃ FET as a function of V_GS. For this purpose we combine standard I_SD-V_GS with C – V_GS. The latter probes the carrier system at the chemical potential and allows us to directly derive the carrier density as a function of V_GS. All experimental data is found to be in excellent agreement with an analytical model based on a 2D electron system over the entire range of V_GS. Most strikingly we find that for our device the values of μ_FE obtained solely from the I_SD – V_GS overestimates those obtained taking into account the measure C – V_GS by more than a factor of ×4.

The sample studied consists of 128°Y-rotated, d = 0.5 mm thick substrate of black lithium niobate (LiNbO₃–d), on top of which a layer of MoS₂ has been deposited by chemical vapour deposition¹⁸,¹⁹. We use such samples for investigations of the interaction of surface acoustic waves with MoS₂, as described in ref.¹⁹.

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a) Electronic mail: wladislaw.michaiłow@gmx.de
b) Electronic mail: hubert.krenner@physik.uni-augsburg.de
the sample backside. A schematic of the sample is shown in Fig. 1. Blue symbols are extracted from the best fits of Eq. (1) to the data in Fig. 1. The error bars represent the statistical errors of the fit.

The sample was characterized by mapping photoluminescence spectroscopy to confirm millimeter-scale growth of MoS2. FET devices were fabricated using an established process19: the MoS2 layer has been removed from the sample surface except of two 0.3 mm × 6.43 mm stripes. This A ≈ 3.86 mm² lithographically defined area includes the regions of highest emission intensity. On top of these stripes, two finger electrodes (10 nm Ti and 60 nm Au) with a distance of 6.37 µm serve as source and drain contacts, contacting the two stripes along their entire 2 × 0.3 mm width. The gate voltage \( V_{GS} \) was applied on the sample backside. A schematic of the sample is shown as inset in Fig. 1. All measurements have been performed under ambient conditions with the device mounted inside a sealed metal chip carrier to exclude any influences of external illumination.

As a first estimate of \( \mu_{FE} \), we measured the source-drain current \( I_{SD} \) at a fixed source-drain voltage \( V_{SD} \) as a function of \( V_{GS} \), as depicted in Fig. 1. For each \( V_{SD} \), a weak hysteresis14 is resolved as the \( V_{GS} \) was scanned \( 0 \rightarrow +40 \text{ V} \rightarrow -40 \text{ V} \rightarrow 0 \text{ V} \), which is less pronounced than that reported for a different sample in our previous work19. The polarity of \( V_{GS} \) is chosen such that \( V_{GS} > 0 \) corresponds to negative charge on the MoS2 layer. These characteristics directly confirm the accumulation of negative charge on the MoS2 layer for \( V_{GS} > 0 \). From this data, we extracted \( V_{Th} \) and \( \mu_{FE} \) using Eq. (1) and the simple parallel-plate capacitor model. The obtained values \( V_{Th} \) and \( \mu_{FE} \) are plotted as a function of \( V_{SD} \) as red symbols in Fig. 2 (a) and (b), respectively. Obviously, both the obtained values and their statistical errors exhibit significant scatter for the different values of \( V_{SD} \). These shortcomings arise from the simple parallel-plate capacitor model and the fact that the \( V_{GS} \)-interval, in which the best fit of Eq. (1) is performed, is chosen by eye in the conducting region, so that all other data is neglected. We note, that this device shows similar characteristics as that reported in our previous work19. In particular, \( \mu_{FE} \) lies in the same range. In order to improve our method, we directly quantify the capacitance between one contact and the back gate as a function of \( V_{GS} \). \( V_{GS} \) is applied as a DC offset gate voltage to the capacitance bridge and modulated with a 1 kHz sine wave by the built-in oscillator. The measured capacitance was corrected for the capacitance of the wires connecting to the sample. In Fig. 3 (a), we plot the obtained capacitance of the sample \( C_{sample} \) (symbols) as a function of \( V_{GS} \). For large negative \( V_{GS} \), \( C_{sample} \) saturates at a constant value of \( C_{sample} = 2.06 \mu \text{F} \). Under these conditions, the MoS2 layer is completely depleted and the measured \( C_{sample} \) corresponds to that of the metal contacts \( C_{contacts} \), which is independent of \( V_{GS} \). As \( V_{GS} \) increases, the surrounding MoS2 2D layer is populated with electrons and the capacitance increases as observed in the data. \( C_{sample}(V_{GS}) \) can be readily described as an equivalent circuit of \( C_{contacts} \) connected in parallel with the \( V_{GS} \)-dependent capacitance of the TMD layer \( C_{MoS2}(V_{GS}) \), shown as an inset of Fig. 3 (a). From \( C_{MoS2}(V_{GS}) = C_{sample}(V_{GS}) - C_{contacts} \) we can directly calculate the electron surface density \( n(V_{GS}) \) on the MoS2 layer by a discrete integration. The symbols in Fig. 3 (b) are the result obtained from

\[
n(V_{GS}) = -\frac{1}{\epsilon \cdot A} \int_{-\infty}^{V_{GS}} C_{MoS2}(V'_{GS})dV'_{GS},
\]

with \( \epsilon \) being the elementary charge. The obtained values for \( n(V_{GS}) \) faithfully reproduce a clear turn-on behavior and linear increase as expected for a FET.

We proceed by developing an analytical model of the \( V_{GS} \)-dependent electron density \( n \). The equilibrium electron density can be calculated by integrating the Fermi distribution function \( f_{FD}(E) = \left( \exp \left( \frac{E - \zeta}{k_B T} \right) + 1 \right)^{-1} \) over
In the top metal contact, the additional electrons accumulate at the position of the electrochemical potential in the gate voltage, leading to a small Schottky barrier, which is built up at the metal–TMD interface. The density of states is determined by the Planck constant, the area of the monolayer, and the Planck constant; the density is counted from the conduction band edge in MoS₂. In the presence of a gate voltage, the chemical potential $\zeta$ in (2) should be modified as $\zeta \rightarrow \zeta + \delta(\zeta(GS))$, where $\delta(\zeta(GS))$ is the shift of $\zeta$ in MoS₂ due to $V_{GS}$. We assume that $\delta(\zeta(GS)) \propto V_{GS}$ and use the following function to fit our experimental data

$$ f(V_{GS}) = a \cdot b \ln \left( 1 + \exp \left( \frac{V_{GS} - V_{Th}}{b} \right) \right), \quad (3) $$

with $V_{Th}$ being a threshold voltage. The result of the best fit of this function to the $n$ derived from the measured capacitance is plotted as the solid line in Fig. 2(b) and shows that this analytical function perfectly follows the experimental data over the entire range of $V_{GS}$.

The values of the parameters $a$ and $b$ extracted from the fit are $a = 2.73 \cdot 10^6 \text{V}^{-1} \cdot \text{cm}^{-2}$ and $b = 10.8 \text{V}$. Since $k_{B}T/e \approx 26 \text{mV}$ we get from $b$ the value of $\alpha \approx 2.4 \cdot 10^{-3}$. Such a small value of $\alpha = \delta(\zeta(GS))/eV_{GS}$ suggests that the density of states is substantially larger than in MoS₂. Indeed, in equilibrium (without gate voltage) a small Schottky barrier is typically built up at the metal–TMD interface. Under these conditions, a certain amount of electrons flow into MoS₂ from the contacts, so that the density $n$ is inhomogeneous and larger in the near-contact areas than in the areas farther away. A positive $V_{GS}$ increases the electron density in the top metal contact. The additional electrons accumulate at the bottom of the contact in a layer with a thickness corresponding to the Thomas-Fermi screening length, which leads to a small increase of the electrochemical potential $\delta(\zeta(GS))$ in the MoS₂–metal contacts system. Due to the high density of states in the metal, $\delta(\zeta(GS))$ is much smaller than $e \cdot U_{G}$, which yields $\alpha \ll 1$. Due to the growth of $\zeta(GS)$, more electrons flow into MoS₂ and larger areas of the 2D semiconductor become well-conducting. This basic physical picture qualitatively agrees with our results.

Comparing the equations (2) and (3), one can see that $a = 2\pi g m^* \cdot e \zeta / h^2$. Using $\alpha$ extracted from $b$ and $m^* \approx 0.45 \cdot m_{e,0}$, one gets $a \approx 9 \cdot 10^{11} \text{V}^{-1} \cdot \text{cm}^{-2}$. In order to explain the deviation from the fit value, a more accurate model is necessary, which takes into account the concrete contact geometry and coordinate dependence.

An analytical expression for the capacitance can be directly obtained by taking the derivative of Eq. (3). We obtain

$$ C(V_{GS}) = (C_{\infty} - C_{\text{contacts}}) \cdot \frac{1}{\exp \left( \frac{V_{Th} - V_{GS}}{b} \right)} + C_{\text{contacts}}, \quad (4) $$

with $C_{\infty}$ being the maximum capacitance for $V_{GS} \rightarrow \infty$. The result of the best fit of Eq. (4) to the measured capacitance is shown as a solid line in Fig. 3 (a) which again faithfully reproduces the experimental data points.

In the next step, we assume that $\mu_{FE}$ is independent of $V_{GS}$. Thus, in the Drude model, $I_{SD}(V_{GS}) \propto n(V_{GS})$ can be fitted using Eq. (3). The results of such best fits for all measured $I_{SD}(V_{GS})$ are plotted as solid lines in Fig. 4 (a). Again, the fitted function faithfully reproduces the experimental data, underlining further the 2DES nature of the conducting channel. Furthermore, these obtained fit functions allow to determine $V_{Th}(V_{SD})$ and $\mu_{FE}(V_{SD})$, using Eq. (1) with $\partial I_{SD}/\partial V_{GS} = 0$ as the slope at large $V_{GS}$, with higher precision. The extracted values for $V_{Th}(V_{SD})$ and $\mu_{FE}(V_{SD})$ are plotted as
blue symbols in Fig. 2 (a) and (b), respectively. Clearly, the scatter of the values derived from the fit results is dramatically reduced. We obtain \( V_{\text{TH}} = (17.0 \pm 0.2) \text{V} \), which is almost constant over the entire range of \( V_{\text{SD}} \). In contrast, \( \mu_{\text{FE}}(V_{\text{SD}}) \) exhibits a clear trend to significantly decrease for increasing \( V_{\text{SD}} \). The negative slope of the \( V_{\text{SD}} \)-dependence of the mobility has its reason in predominantly in hysteresis and drifts of the electrical characteristics. Both effects are commonly observed in such devices\(^{14,20}\).

Finally, we turn to carrier mobility and its dependence on the gate voltage, \( \mu_{\text{FE}}(V_{\text{GS}}) \). In the Drude model the conductivity is given by \( \sigma = e \cdot n \cdot \mu_{\text{FE}} \). Thus, the mobility given by \( \mu_{\text{FE}}(V_{\text{GS}}) = \sigma(V_{\text{GS}})/(e \cdot n(V_{\text{GS}})) \) can be calculated only from measured data: \( \sigma(V_{\text{GS}}) \) can be derived from the \( I_{\text{SD}}(V_{\text{GS}}) \) characteristics [Figs. 1 and 4 (a)] and \( n(V_{\text{GS}}) \) from the \( C_{\text{MoS}_2}(V_{\text{GS}}) \) data [cf. Fig. 4 (b)]. We note that this analysis can be performed for our data only for \( V_{\text{GS}} \gtrsim 0 \text{V} \). For negative \( V_{\text{GS}} \) both \( \sigma \) and \( n \) vanish and any obtained value of \( \mu_{\text{FE}} \approx \sigma/n \) exhibits a large error. In Fig. 2 (b) we plot \( \mu_{\text{FE}}(V_{\text{GS}}) \) obtained directly from the measured (symbols) and the fitted (lines) \( I_{\text{SD}}(V_{\text{GS}}) \) characteristics for different values of \( V_{\text{SD}} \) for \( V_{\text{GS}} > 0 \text{V} \). Remarkably, the absolute value of \( \mu_{\text{FE}} \) shown in Fig. 4 (b), which we obtained by including measured, realistic capacitance (and thereby \( n \)) data is significantly lower than that obtained from the basic parallel-plate capacitor model [cf. Fig. 2 (b)]. It ranges between \( \mu_{\text{FE}}(V_{\text{GS}}) \sim 4 \pm 10 \text{cm}^2\text{V}^{-1}\text{s}^{-1} \) and shows a pronounced increase with increasing \( V_{\text{GS}} \) (in addition to its global reduction as \( V_{\text{SD}} \) reduces [cf. Fig. 2 (b)]). For \( 0 < V_{\text{GS}} < V_{\text{TH}} \), \( \mu_{\text{FE}} \) rapidly increases as the injected electrons screen scattering centers in the channel. Such behavior is well established and has been observed for 2DES in established III-V semiconductor heterostructures\(^{21,22}\). For \( V_{\text{GS}} > V_{\text{TH}} \) this trend weakens and \( \mu_{\text{FE}} \) saturates. This saturation behavior can be readily understood considering that as the chemical potential \( \zeta \) is fully shifted into the conduction band. For large positive \( V_{\text{GS}} \) the chemical potential lies well above the random potential modulation induced by scattering centers. Thus, any further increase of \( \zeta \) (i.e. \( n \)) does not lead to improved screening and, thus increased \( \mu_{\text{FE}} \).

In summary, we demonstrated that combined electrical transport \( (I_{\text{SD}} - V_{\text{GS}}) \) and capacitance \( (C - V_{\text{GS}}) \) spectroscopy allows to determine the field-effect mobility \( \mu_{\text{FE}} \) and threshold voltage \( V_{\text{TH}} \) of a TMD based FET with significantly higher precision than the commonly applied basic parallel-plate capacitor model. We performed a three step analysis on model data of a MoS\(_2\)-LiNbO\(_3\) FET device starting with the basic parallel-plate capacitor model. For our device the \( V_{\text{GS}} \)-dependent \( I_{\text{SD}} \), \( n \) and \( C \) are in excellent agreement with an analytical model of an ideal 2DES over the entire range of \( V_{\text{GS}} \). This is in strong contrast to the basic parallel-plate capacitor model in which only data in a small, subjectively chosen interval of the \( I_{\text{SD}} - V_{\text{GS}} \)-characteristics is considered. The statistical errors of \( \mu_{\text{FE}} \) and \( V_{\text{TH}} \) can be significantly reduced by fitting and evaluating the \( I_{\text{SD}} - V_{\text{GS}} \)-characteristics using our 2DES model as now the full data range is included. Finally, by including the full \( C - V_{\text{GS}} \)-characteristics and the derived carrier density \( n \) we are able to obtain the \( V_{\text{GS}} \)-dependent \( \mu_{\text{FE}} \).

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