

Challenges of Drift-Diffusion Simulation for Device Characterization at 4.2 K

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Abstract—Semiconductor device simulation based on the drift-diffusion model is used to analyze measurement data of an nMOSFET at cryogenic temperatures. The simulation is complicated by nonlinearities which emerge at lower bias and smaller signal swings than at room temperature. We demonstrate that saturation is not negligible even at low drain-source voltages and that small-signal measurements leave the linear regime already at very small AC amplitudes. Ignoring these effects can lead to erroneous interpretations of measurement data, especially close to the threshold voltage.

Index Terms—Cryogenic electronics, drift-diffusion model, large-signal simulation, inversion layer mobility

I. INTRODUCTION

Operating MOSFETs at 4.2 K or below not only allows co-integration with quantum computing qubits but also promises performance gains due to the potentially extremely steep subthreshold slope and increased mobility. However, before these merits can be utilized technologically, our physical understanding needs to improve significantly. The only way to achieve this is with an interplay between simulation and measurement, because standard test structures (e.g. lightly doped MOS caps) fail due to, for example, impurity freezeout. Instead, more complex structures such as MOSFETs should be considered.

In this work, n-type bulk Si MOSFETs have been characterized at cryogenic temperatures. Devices with a very large area have been fabricated to enable both current-voltage and admittance spectroscopy measurements with a good signal-to-noise ratio (SNR). The experimental results were used to calibrate an in-house drift-diffusion simulator which can handle the well-known numerical difficulties [1] at such extreme temperatures. 3D simulations were conducted which include Fermi-Dirac statistics without approximations and models for impurity freezeout and band-tailing. The simulation results indicate strong nonlinearities in the device behavior which make device characterization based on approximate formulas or linearization inaccurate. Instead, full device-scale simulations should be used at cryogenic temperatures to ensure that measurement data are interpreted correctly.

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II. METHODOLOGY

A. Device Fabrication and Measurement

We consider a large area nMOSFET with $W/L = 2172\mu\text{m}/80\mu\text{m}$ and substrate doping $N_A = 7 \times 10^{14}\text{cm}^{-3}$. The gate oxide is 22 nm HfO_2 below which an ultrasMOOTH 0.9 nm SiO_2 layer was added according to the process described in [2] in order to decrease interface microroughness and the density of localized defect states at the interface. The source, gate and drain contacts each include four bond pads which are connected to the main electrode via narrow connections. In the case of the gate contact, these bond pads are placed on the same oxide as the main electrode such that their influence is non-negligible, making 3D simulations necessary. A photo of one half of the symmetric device is shown in Fig. 1, more details on the layout are given in [3].

The admittance spectroscopy measurements have been recorded at 4.2 K with a HP 4284A Precision LCR Meter with 28 mV amplitude leaving the drain contact floating. The transfer characteristics were measured at different temperatures using a Keithley 4200-SCS parameter analyzer.

B. Drift-Diffusion Simulation

The drift-diffusion equations are discretized using the finite volume method. The solver includes Fermi-Dirac statistics without approximations by utilizing the generalized Scharfetter-Gummel stabilization scheme from [4]. Incomplete ionization is included based on the equations from [3] to which terms accounting for field-enhanced ionization (tunneling and Poole-Frenkel effect) were added. The highly doped source and drain regions ($N_D \approx 10^{20}\text{cm}^{-3}$) are assumed to be fully ionized [5]. Overall, the solution variables in the system are the electrostatic potential, the particle densities, the concentration of ionized acceptors and the contact currents. Transient simulations are performed using TR-BDF2 [6] with adaptive time steps. As opposed to small-signal simulations, in the transient case the influence of the floating drain contact cannot be included via post-processing, leading to additional numerical difficulties similar to the floating body effect.

Disorder at the interface and other effects induce additional states in the bandgap, leading to the formation of a band-tail in the density of states (DOS). This effect has a major impact on the device performance at cryogenic temperatures as it determines the limit of the subthreshold swing [7]. The

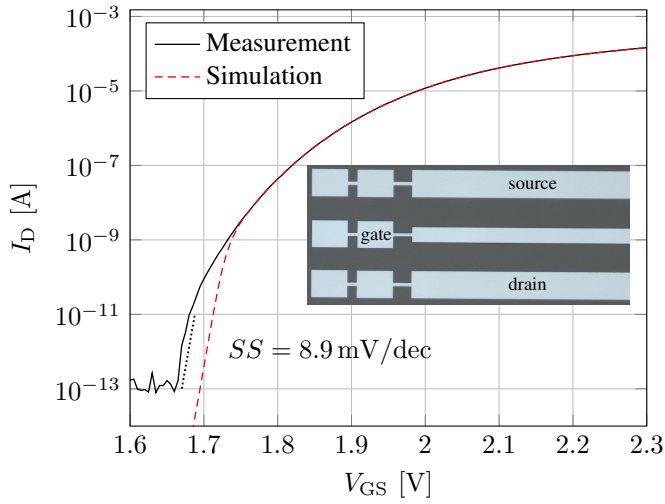


Fig. 1: Measured and simulated transfer characteristic at $V_{DS} = 100$ mV and $T = 4.2$ K. The subthreshold swing of the simulation is matched to the first two decades above the noise floor of the measured I_D . The inset shows one half of the symmetric device including the bond pads.

band-tail is frequently modeled to be exponentially decaying. When the DOS is additionally required to be continuously differentiable, this leaves the characteristic decay energy as the only free parameter and results in the DOS given in [3, 4], which is also used here for the electrons. For the holes, we use a parabolic band structure.

The analysis of the influence of localized interface traps is beyond the scope of the present work. Therefore, these states are not directly included in the simulation. Their main influence is expected to be an increase of the threshold voltage and a degradation of the subthreshold swing around the threshold voltage, which we include indirectly by adjusting the metal-semiconductor workfunction difference ϕ_{MS} and the inversion layer mobility, respectively.

C. Parameter Calibration and Extraction

To reduce uncertainties in the model, some of the device specifications were verified with additional measurements. This includes laser microscopy for the exact sizes of the metal contacts, electrochemical capacitance-voltage (ECV) measurements for the doping profile and temperature-dependent transfer length method (TLM) measurements for the resistance of the source/drain regions R_S .

The permittivity of the gate stack is extracted from a capacitance measurement in inversion.

Fabrication tolerances can lead to an offset of the gate electrode with respect to the ohmic source/drain regions. This impacts the capacitance especially in depletion where it is dominated by the overlap. The offset distance used for the simulations can thus be obtained by matching the depletion capacitance C_{dep} .

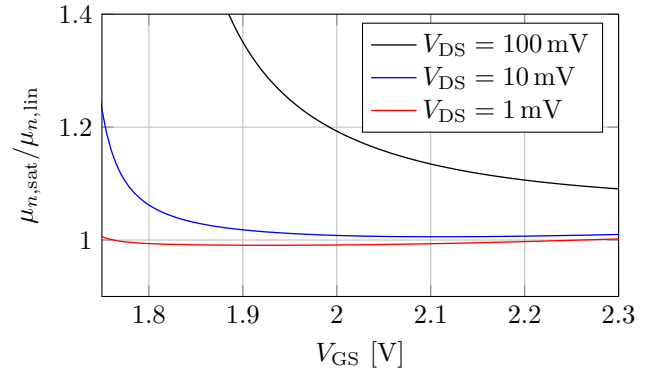


Fig. 2: Deviation of the inversion layer mobility calculated with Eq. (2) from the mobility obtained by matching the 2D drift-diffusion simulation at 4.2 K.

To obtain the characteristic decay energy of the band-tail E_{bt} , at first the measured subthreshold swing SS just above the noise floor is determined, which is about 8.9 mV/dec (dotted line in Fig. 1). This value can be translated into E_{bt} via [7]

$$SS \Big|_{k_B T \ll E_{bt}} = m \frac{E_{bt}}{e} \ln(10) \quad (1)$$

where k_B is the Boltzmann constant and e the elementary charge. m is a slope factor which mainly depends on the gate stack and is close to unity for the device considered here. In our case, we end up with $E_{bt} = 3.8$ meV.

The electron mobility in the ohmic source/drain regions is set such that R_S in the simulations matches the TLM measurements. In the inversion layer, the mobility depends on the gate voltage and can be extracted by iteratively matching the measured and simulated transfer characteristic (cf. Fig. 1). For the simulation of the transfer characteristic, a suitable ϕ_{MS} has to be chosen beforehand and the drift-diffusion model has to be solved in at least 2D.

At cryogenic temperatures, this process cannot be simplified by using formulas which neglect saturation [8] like

$$\mu_n = I_D L / (e N_{inv} W (V_{DS} - 2 R_S I_D)) \quad (2)$$

with the inversion density N_{inv} . Close to the threshold where saturation is not negligible this approach leads to drastic underestimation of the mobility by a factor of two or more, as can be seen in Fig. 2. Even for V_{DS} as small as 10 mV, the error close to the threshold voltage is beyond 10 %. As V_{DS} cannot be chosen arbitrarily small due to measurement SNR constraints, it is necessary to use full device simulations for characterization.

In Fig. 1 it is visible that the measured subthreshold swing is not constant but degrades toward the threshold voltage. This effect is known as inflection and is attributed to a distribution of localized states close to the band edge [9]. As a model for interface states is beyond the scope of this paper, the effect is only included indirectly by fitting the subthreshold mobility. Therefore, the extracted mobility is only

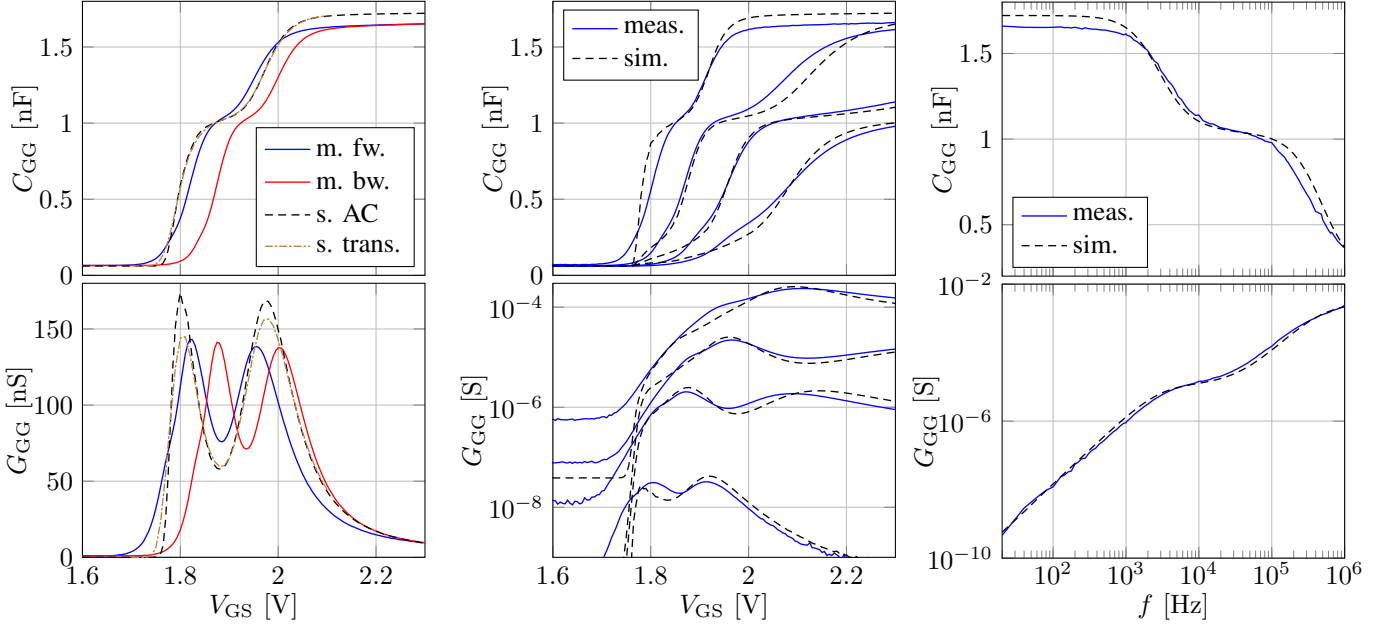


Fig. 3: Simulated and measured gate capacitance and conductance at different voltages, frequencies and 4.2 K, where the drain contact is open.

quantitatively meaningful above the threshold voltage where the influence of the localized states is negligible.

Overall, the model parameters of primary importance are the source/drain region mobility (obtained from R_S), the oxide permittivity (obtained from C_{inv}), the gate offset (obtained from C_{dep}), E_{bt} (obtained from SS), and the inversion layer mobility and ϕ_{MS} (both obtained from fitting). They are used for subsequent small-signal (Fig. 3) and transient (Fig. 4) simulations. The measurements exhibit a drift of the threshold voltage across different tests for the same device, as can be seen for example in the shift between forward and backward voltage sweep in Fig. 3a. The drift is likely caused by charges entering the oxide due to the applied bias. In the simulation, this has to be accounted for by a slight adjustment of ϕ_{MS} . The gate conductance was not used for any parameter fitting and can therefore serve as a benchmark of the agreement between simulation and measurements.

III. RESULTS

The gate capacitance and conductance obtained by simulations are compared to the measurement results over a wide range of frequencies and gate voltages in Fig. 3. The capacitance increases in two steps when either the frequency is decreased (Fig. 3c) or the gate voltage is increased (Fig. 3a). This is caused by the device geometry with the non-negligible bond pads which are connected to the main gate electrode via a narrow connection (cf. Fig. 1) resulting in a relatively

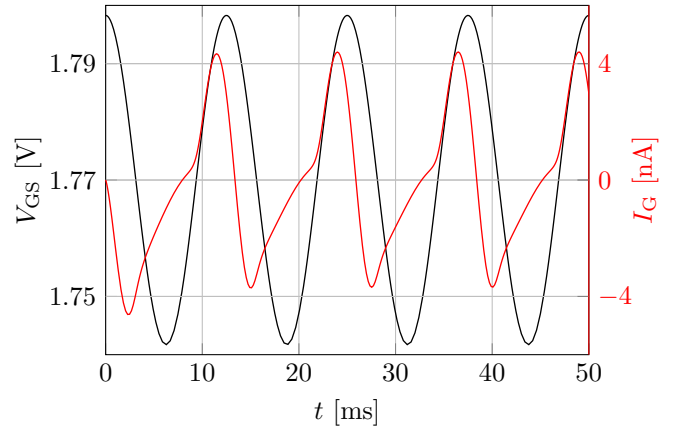


Fig. 4: Simulated gate current when applying an AC voltage of 28 mV at $V_{GS,DC} = 1.77 \text{ V}$, $f = 80 \text{ Hz}$, $T = 4.2 \text{ K}$.

high resistance between the inversion layers in the channel and beneath the bond pads. This shifts the capacitance contribution of the bond pads toward lower frequency / higher gate voltage [3]. The geometry also influences the gate conductance which exhibits a pattern with two distinct peaks. In the subthreshold region, the measured conductance tends toward an unexpectedly high value caused by unknown sources outside the channel. This is not captured in the simulation, but above the threshold voltage the agreement between simulation and

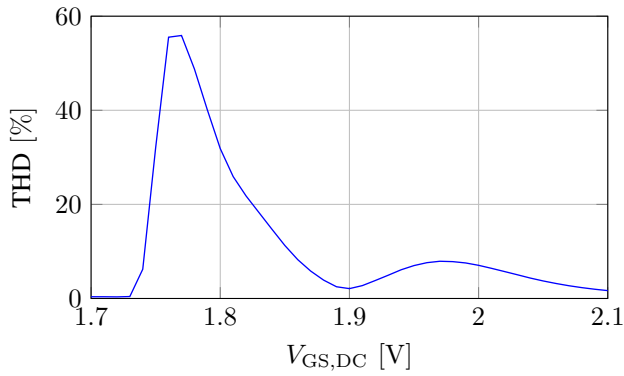


Fig. 5: Voltage-dependent total harmonic distortion of I_G at $V_{GS,AC} = 28 \text{ mV}$, $f = 80 \text{ Hz}$, $T = 4.2 \text{ K}$.

measurement is good.

The analysis of the admittance spectroscopy data is further complicated by the shrinking of the linear response region at cryogenic temperatures. The measurement data at 4.2 K have been recorded using an AC amplitude of 28 mV which is a comparably small amplitude. But it is still much larger than the thermal voltage and the device already operates beyond the linear response regime. This can be verified by transient simulation results as in Fig. 4 where I_G is clearly nonlinear. As a measure of nonlinearity, the total harmonic distortion (THD) of I_G at $f = 80 \text{ Hz}$ depending on $V_{GS,DC}$ is shown in Fig. 5. Nonlinearity is especially high close to the threshold voltage, but even at higher voltages it exceeds 7 %. This can cause large errors when calculating gate capacitance and conductance based solely on small-signal simulations which are linear by definition. This can be seen in Fig. 3a where the small-signal simulation results are compared to the capacitance and conductance calculated from transient simulations. Deviations occur especially in the gate conductance at the abrupt transition near the threshold and near the extrema. Unfortunately, using transient simulations for each data point at each frequency is not feasible due to long simulation duration. The small-signal simulations still provide a good estimate, but it is important to keep in mind that they cannot reproduce nonlinearities in the measurement data.

Using the procedure described above, we furthermore extracted the electron inversion layer mobilities at different temperatures from measurements. The results in Fig. 6 indicate that at low effective fields the mobility rises with temperature. At higher effective fields, the dependency is reversed and the highest mobilities are obtained at the lowest temperature. This behavior was reported as well in [3].

IV. CONCLUSION

Measurement data of an nMOSFET at cryogenic temperatures were analyzed using drift-diffusion simulations. Two sources of nonlinearities were identified which complicate the interpretation of the measurement data. First, the mobility cannot be analyzed without including saturation, at least for

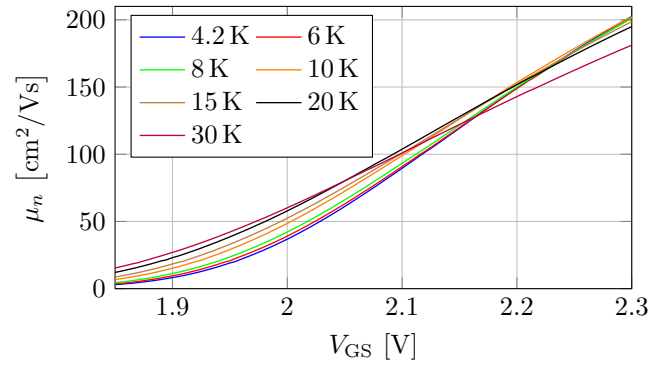


Fig. 6: Extracted electron inversion layer mobilities at different temperatures.

typical V_{DS} used in measurement. Second, small-signal measurements leave the linear response regime much sooner than at room temperature which can lead to significant deviations in the admittance spectroscopy measurements close to the threshold voltage. To include these effects in the simulation, at least 2D simulations of the full drift-diffusion model are necessary. Due to the complex device geometry, in this work we had to use 3D simulations where we achieved a good agreement with the measurement data.

REFERENCES

- [1] M. Kantner and T. Koprucki, "Numerical simulation of carrier transport in semiconductor devices at cryogenic temperatures," *Optical and Quantum Electronics*, vol. 48, no. 12, p. 543, Nov 2016. [Online]. Available: <https://doi.org/10.1007/s11082-016-0817-2>
- [2] Y.-C. Chang, M. Motylenko, Y.-T. Liao, J. Sun, M. Kasavetov, V. Rincón Montes, Q.-T. Zhao, D. Rafaja, and J. Knoch, "Ultrasoft sub-nanometer chemical SiO₂ surfaces and enhanced interface characteristics via high-ph fluoride treatment for Si/HfO₂ MOS devices," *ACS Applied Materials & Interfaces*, vol. 18, no. 10, pp. 15 721–15 734, 2026, pMID: 41780992. [Online]. Available: <https://doi.org/10.1021/acsami.5c23465>
- [3] C. Jungemann, B. Richstein, T. Linn, and J. Knoch, "Device modeling for admittance spectroscopy of PMOSFETs at cryogenic temperatures," *IEEE Transactions on Electron Devices*, vol. 71, no. 4, pp. 2322–2328, 2024.
- [4] T. Linn, M. Renner, and C. Jungemann, "Thermodynamically consistent stabilization of the drift-diffusion model for arbitrary band structures and carrier statistics," *Journal of Computational Electronics*, vol. 24, no. 6, p. 171, Sep 2025. [Online]. Available: <https://doi.org/10.1007/s10825-025-02412-4>
- [5] P. P. Altermatt, A. Schenk, and G. Heiser, "A simulation model for the density of states and for incomplete ionization in crystalline silicon. I. establishing the model in Si:P," *Journal of Applied Physics*, vol. 100, no. 11, p. 113714, 12 2006. [Online]. Available: <https://doi.org/10.1063/1.2386934>
- [6] R. E. Bank, W. M. Coughran, JR., W. Fichtner, E. H. Grosse, D. J. Rose, and R. K. Smith, "Transient simulation of silicon devices and circuits," *IEEE Trans. Computer-Aided Des.*, vol. 4, pp. 436–451, 1985.
- [7] A. Beckers, F. Jazaeri, and C. Enz, "Theoretical limit of low temperature subthreshold swing in field-effect transistors," *IEEE Electron Device Letters*, vol. 41, no. 2, pp. 276–279, 2020. [Online]. Available: <https://doi.org/10.1109/LED.2019.2963379>
- [8] S. M. Sze, *Physics of Semiconductor Devices*. New York: Wiley, 1981.
- [9] A. Beckers, F. Jazaeri, and C. Enz, "Inflection phenomenon in cryogenic MOSFET behavior," *IEEE Transactions on Electron Devices*, vol. 67, no. 3, pp. 1357–1360, 2020. [Online]. Available: <https://doi.org/10.1109/TED.2020.2965475>