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High-temperature modeling of AlGaN/GaN HEMTs

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ABSTRACT

Wide bandgap, high saturation velocity, and high thermal stability are some of the properties of GaN, which make it an excellent material for high-power, high-frequency, and high-temperature applications. As several application areas require the devices to operate at elevated temperatures, a proper modeling of the temperature dependences of the band structure and transport parameters is very important. We present two-dimensional hydrodynamic simulations of AlGaN/GaN high electron mobility transistors (HEMTs) at high temperatures. The simulator is calibrated against measurement data of a real device and delivers good predictive results for the DC and RF characteristics of another. The temperature dependence of the maximum current and cut-off frequency of submicron devices is further studied.

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1. Introduction

GaN takes advantage of the interesting material properties of the III-nitrides, such as a wide bandgap (3.4 eV), high breakdown electric field (4 MV/cm) and excellent thermal conductivity [1]. The latter two make GaN an interesting candidate for high-temperature systems. On the other hand, the high electron mobility (1600 cm²/Vs) and high saturation velocity ($v_{\rm sat} > 1.5 \times 10^7$ cm/s) give GaN an edge over other wide bandgap materials, as they allow RF operation of the devices. Consequently, outstanding results for the power density in GaN HEMTs have been reported in the last few years, e.g. 8.6 W/mm at the Ka-band [2] and 40 W/mm at the C-band [3], and the devices are considered for high-power high-frequency applications at elevated temperatures [4].

Several groups have studied the high-temperature DC operation of AlGaN/GaN HEMTs on different substrates (sapphire [5–7], SiC [6] and Si [7,8]).

AC measurements at elevated temperatures however are sparse: e.g. the temperature dependence of the cut-off frequency is compared to that of the transconductance by Akita et al. [9]. An investigation of the influence of high temperature on the microwave power performance of AlGaN/GaN HEMTs is conducted by Arulkumaran et al. [10].

On the other hand, the theoretical studies of GaN-based transistors at higher temperature are also rare. There are few analytical models developed [11–13], however those are tailored for use in

circuit simulation, not for device optimization. To our knowledge there is only one work, which focuses solely on high-temperature HEMT device simulation [14], however it relies on dated experimental data [9] and does not feature AC performance.

In the subsequent study the material and model parameters for GaN and AlGaN are discussed. They are incorporated in the two-dimensional device simulator Minimos-NT [15]. The simulator is then calibrated against measurement data of a state-of-the-art $l_{\rm g}$ = 0.25 μ m device at room and elevated temperatures. Using the same set of models and parameters predictive simulations for a $l_{\rm g}$ = 0.5 μ m device are conducted. Good agreement for the DC and AC characteristics is achieved. Further, the temperature dependence of the drain current and cut-off frequency on the gate length is theoretically studied for sub-quartermicron devices.

2. Physical and material models

We perform two-dimensional hydrodynamic electro-thermal simulations with our device simulator Minimos-NT, which proved to be a suitable tool for the analysis of heterostructure devices [16]. We have used it for the optimization of field-plate structures [17] and the design of new device generations [18].

Our choice of transport model aims to achieve maximum accuracy combined with computational efficiency. Since the drift-diffusion transport model is not able to deliver accurate results for submicron GaN FETs [19,20], we employ the hydrodynamic transport model. As AlGaN/GaN HEMTs are unipolar devices, computational effort is reduced by neglecting the equations for holes in this work. Self-heating effects are accounted for by the lattice heat flow equation. It is obtained from the stationary energy flux balance derived

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from the second moment solving the Boltzmann transport equation and the carrier continuity equation. The heat generation is expressed as the sum of the energy relaxation approximation of the scattering terms of the Boltzmann equation and the effective recombination. The hydrodynamic transport model is derived from the Boltzmann equation by taking into account the first four moments of the distribution function. In order to obtain a closed equation set the heated Maxwellian distribution is assumed [21]. A macroscopic relaxation time approximation is used.

Finally, a system of four partial differential equations: Poisson, current continuity and energy balance for electrons, and the lattice heat flow equation, is solved self-consistently. For the heat flow, Neumann boundary conditions are assumed at all device boundaries. The only exception is the bottom boundary, where an additional thermal contact is introduced, which models the heat flow into the substrate. The lattice temperature is calculated using a specified contact temperature (equal to the ambient temperature in our simulations) and a thermal resistance. The latter represents the lumped thermal resistance of the nucleation layers and the substrate. The thermal heat-flow across the boundary is accounted for self-consistently.

The four differential equations have material-specific parameters, such as bandgap energy, electron mobility, thermal conductivity, etc. The dependence of these parameters on temperature, energy, etc. is described by models, which are presented in the following.

2.1. Bandgap energy

The Varshni formula describes well the temperature dependence of the band gap in nitrides. The temperature dependence of the bandgap is calculated by:

$$E_{\rm g} = E_{\rm g,0} - \frac{\alpha_{\rm g} T_{\rm L}^2}{\beta_{\rm g} + T_{\rm L}}.$$

The values for $E_{\rm g,0}$ (energy band gap at 0 K), $\alpha_{\rm g}$ and $\beta_{\rm g}$ (empirical constants) for GaN and AlN are shown in Table 1. The parameter values for GaN are an average of various reported results as summarized in [22], while those for AlN are based on the experimental work of Guo et al. [23]. The bandgap of $Al_xGa_{1-x}N$ is then interpolated by:

$$E_{\mathrm{g}}^{AlGaN} = E_{\mathrm{g}}^{AlN}(1-x) + E_{\mathrm{g}}^{GaN}x + C_{\mathrm{g}}(1-x)x,$$

with the bowing parameter C_g . The reported values of the latter show a large variation ranging from -0.8 [24] to 1.33 [25]. However, several experiments [26,27] show a linear variation ($C_g \approx 0$), which is adopted here.

An energy offset (E_{off}) is used to align the valence band of different materials. For Al_xGa_{1-x}N it is calculated by:

$$E_{\rm off}^{\rm AlGaN} = \frac{E_{\rm off}^{\rm AlN} \left(E_{\rm g}^{\rm AlGaN} - E_{\rm g}^{\rm GaN}\right) - E_{\rm off}^{\rm GaN} \left(E_{\rm g}^{\rm AlGaN} - E_{\rm g}^{\rm AlN}\right)}{E_{\sigma}^{\rm AlN} - E_{\sigma}^{\rm GaN}}, \label{eq:energy}$$

where $E_{\rm off}^{\rm GaN}$ and $E_{\rm off}^{\rm AlN}$ are the offset energies for GaN and AlN, respectively. As the valence band edge of GaN is chosen as reference, $E_{\rm off}^{\rm GaN}$ is set to 0 eV. The valence-band-offset of AlN $E_{\rm off}^{\rm AlN}$ is chosen as 1.12 eV, which is equal to 40% of the total bandgap discontinuity as reported by Westmeyer et al. [28]. For $Al_xGa_{1-x}N$ with x=0.22,

Table 1Summary of band structure parameters.

Material	E _{g,0} (eV)	α _g (eV/K)	β _g (K)
GaN	3.4	$\begin{array}{c} 9.09 \times 10^{-4} \\ 18.0 \times 10^{-4} \end{array}$	800
AlN	6.2		1462

the valence-band-offset against GaN is 0.25 eV (further, our setup provides a value of 0.225 eV for x = 0.2, which is in a good agreement with the experimentally determined offset of 0.25 eV [29] for the same composition). We have experimentally determined the barrier height of the Schottky contact to GaN to be 1.0 eV at room temperature in agreement with experiments by other groups [30]. The changes in the barrier height with temperature (in the range under investigation) are negligibly small [31].

2.2. Spontaneous and piezoelectric polarization

A good understanding of the electrical polarization effects at the $Al_xGa_{1-x}N/GaN$ interface is a key to the proper device simulation. The spontaneous polarization P_{SP} and the strain-induced piezoelectric polarization P_{PZ} are calculated by:

$$\begin{split} P_{\text{SP}} &= P_{\text{SP,AIN}} + P_{\text{SP,GaN}}(1-x), \\ P_{\text{PZ}} &= 2 \cdot \frac{a-a_0}{a_0} \bigg(e_{31} - e_{33} \cdot \frac{C_{13}}{C_{33}} \bigg), \end{split}$$

where a and a_0 are the lattice constants, e_{13} and e_{33} are the piezoelectric coefficients, C_{13} and C_{33} denote the elastic constants. The methodology and the parameter values are after [32,33]. The total polarization-induced sheet charge density at the Al_{0.22}-Ga_{0.78}N/GaN interface calculated by using these expressions is $1.23 \times 10^{13} \ \mathrm{cm}^{-2}$. In the real device however, several effects (such as dislocations or surface states) can significantly reduce this value. Therefore, after calibration against the measurement data, we adopt a sheet charge density of $9.5 \times 10^{12} \ \mathrm{cm}^{-2}$ at the channel/barrier interface and a complementary charge density of $-2.5 \times 10^{12} \ \mathrm{cm}^{-2}$ at the barrier/cap interface.

The dependence of the spontaneous polarization coefficients for GaN and AlN on temperature has been measured to be minimal [33,34]. There are also no reports on the piezoelectric polarization at higher temperatures. Hence, we retain the same sheet charge density values for higher temperatures too.

2.3. Thermal conductivity

The thermal conductivity is modeled by a power law:

$$\kappa(T_{\rm L}) = \kappa_{300} \cdot \left(\frac{T_{\rm L}}{300 \text{ K}}\right)^{\alpha},$$

where κ_{300} is the value at 300 K. From early experiments, a κ_{300} = 130 W/mK for 'bulk' GaN [35] was extracted. However, later measurements of epitaxial structures yielded higher values [36], and a strong dependence on the dislocation density was observed [37]. Based on various studies [35,36,38–41] we give two parameter sets in Table 2, applicable for different material quality. Fig. 1 compares the two model sets with other models and experimental data (model 1 is used in the simulations). For AlN the variation of the measured values for the thermal conductivity is smaller (Fig. 2). We assume a κ_{300} of 350 W/mK, which is close to the value reported by [42]. The parameter α , which models the decrease with temperature is calibrated against measured data [42–44].

Table 2Summary of thermal properties.

Material	κ ₃₀₀ (W/m K)	α
GaN model 1	130	-0.43
GaN model 2	220	-1.2
AlN	350	-1.7

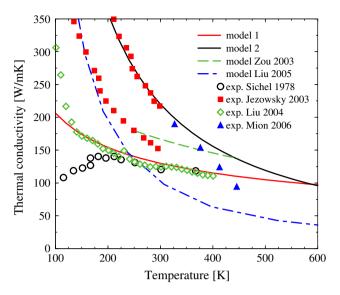


Fig. 1. GaN thermal conductivity as a function of temperature.

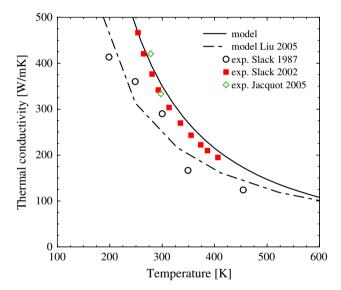


Fig. 2. AlN thermal conductivity as a function of temperature.

2.4. Mobility model

The low-field mobility is modeled by an expression similar to that proposed by Caughey and Thomas [45,16]:

$$\mu^{\text{LI}} = \mu^{\text{min}} + \frac{\mu^{\text{L}} - \mu^{\text{min}}}{1 + \left(C_{\text{I}}/C^{\text{ref}}\right)^{\gamma_0}} \,. \label{eq:multiple}$$

 $C_{\rm I}$ denotes the concentration of ionized impurities, $\mu^{\rm L}$ is the mobility in undoped material, $\mu^{\rm min}$ is the mobility in highly doped material, limited by impurity scattering. In order to model the temperature dependence the mobilities are additionally parameterized using power laws:

$$\mu^{\text{L}} = \mu^{\text{L}}_{300} \Big(\frac{T_{\text{L}}}{300 \, \text{K}} \Big)^{\gamma_1}, \quad \mu^{\text{min}} = \mu^{\text{min}}_{300} \Big(\frac{T_{\text{L}}}{300 \, \text{K}} \Big)^{\gamma_2}.$$

Similar expressions have been used also by others [46,47]. To calibrate the γ_1 and γ_2 parameters we rely on our own Monte Carlo

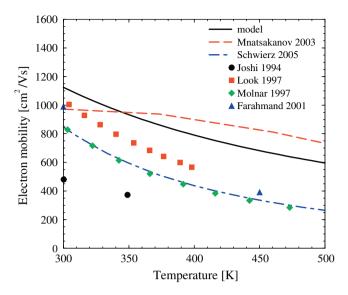
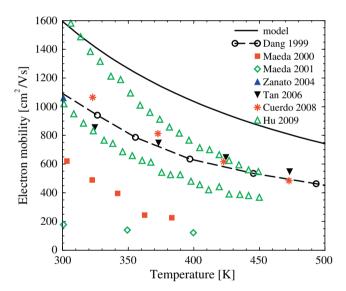


Fig. 3. Low-field bulk mobility in GaN as a function of lattice temperature.



 $\label{eq:Fig.4.} \textbf{Fig. 4.} \ \ \text{Low-field 2DEG mobility at the AlGaN/GaN interface as a function of lattice temperature.}$

simulation, which consider a high-quality material [48]. Monte Carlo (MC) simulations by other groups [46,49] and experiments [50,51] for the electron mobility in bulk GaN as a function of the temperature are shown in Fig. 3. Over the years the electron mobilities increase due to the improved quality of the material samples. Models proposed by other groups [47,52] are also displayed. Fig. 4 shows the electron mobility as a function of temperature in the two-dimensional electron gas (2DEG) as experimentally determined by various groups [53–57,8]. The 2DEG mobility exhibits overall higher values especially at high temperatures, while retain-

Table 3Summary of low-field mobility model parameters for GaN.

$\mu_{300}^{ ext{L}}$	$\mu_{300}^{ m min}$	γο	γ1	γ ₂
1600 cm ² /Vs	100 cm ² /Vs	0.065	-1.5	-0.2

ing the trend for improved results over time. The parameter values we choose are listed in Table 3. The maximum $(\mu^{\rm L}_{300})$ and minimum mobility $(\mu^{\rm min}_{300})$ are calibrated against our own MC simulation. A decrease of the maximum mobility with temperature $(\gamma_1 = -1.5)$, in agreement with the power term of the acoustic phonon mobility expression [58] is assumed. Our MC simulation results and recent experiments from [59] confirmed that the latter is the dominant scattering mechanism at high temperatures. A weak temperature dependence $(\gamma_2 = -0.2)$ of the electron mobility at high concentrations is adopted.

A two-valley hydrodynamic mobility model describes the high-field electron transport. It is derived from the high-field mobility model using the local energy balance equation:

$$\begin{split} & \mu_{\mathrm{v}}(T_{\mathrm{n}}) = \frac{2 \cdot \mu_{\mathrm{v}}^{\mathrm{LL}}}{2 + a_{\mathrm{v}} + \sqrt{a_{\mathrm{v}} \cdot (4 + a_{\mathrm{v}})}}, \quad \mathrm{v} = \Gamma, U, \\ & a_{\mathrm{v}} = \frac{3 \cdot \mathrm{k_{B}} \cdot \mu_{\mathrm{v}}^{\mathrm{LL}} \cdot (T_{\mathrm{n}} - T_{\mathrm{L}})}{2 \cdot \mathrm{q} \cdot \tau_{\mathrm{v}} \cdot (\nu_{\mathrm{sat,v}})^{2}}, \end{split}$$

where $\mu_{\rm v}^{\rm LI}, \tau_{\rm v}$, and $v_{\rm sat,v}$ are the valley-specific low-field mobilities, relaxation times, and saturation velocities. A weighted mean is then built:

$$\mu = \frac{\mu_{\Gamma} + \mu_{U} \cdot P_{U}}{1 + P_{U}}.$$

The coefficient P_U defines the dominant mobility (μ_{Γ} is the mobility in the lowest Γ valley, μ_U is the mobility in the next ML valley) dependent on the valley occupancy:

$$\label{eq:pu} \textit{P}_{\textrm{U}} = 6 \cdot \left(\frac{m_{\textrm{U}}^*}{m_{\textrm{T}}^*} \right)^{3/2} \cdot exp \left(-\frac{\Delta \textit{E}_{\textrm{C}}}{k_{\textrm{B}} \cdot T_{\textrm{n}}} \right) .$$

 $m_{\rm U}^*$ and $m_{\rm \Gamma}^*$ are the electron masses in the respective valleys, $T_{\rm n}$ the electron energy.

The model delivers an acceptable approximation in comparison to MC simulations, accounting for six bands [58] (Fig. 5). Results from different groups vary largely (e.g. peak velocity from 2.5×10^7 cm/s to 3.5×10^7 cm/s), therefore our goal is not a perfect agreement with this particular MC simulation. The model is a carefully chosen trade-off. It provides a velocity-field characteristics close to the one obtained by MC simulation on the one hand,

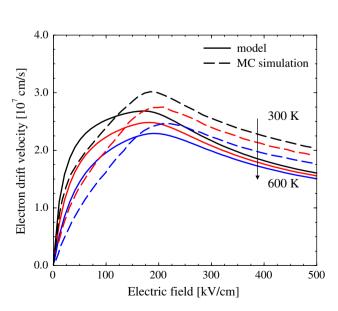


Fig. 5. Electron drift velocity versus electric field for lattice temperature of 300, 450 and $600\ K$.

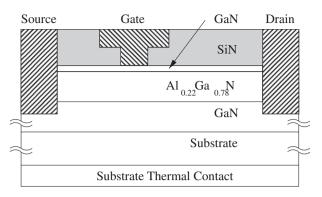


Fig. 6. Schematic layer structure of the investigated device.

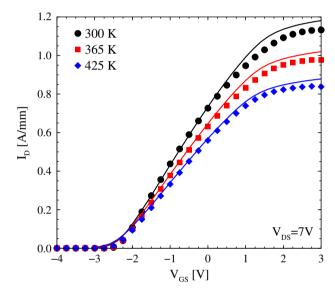


Fig. 7. Calibrated transfer characteristics versus experimental data (symbols) for l_σ = 0.25 μm HEMT.

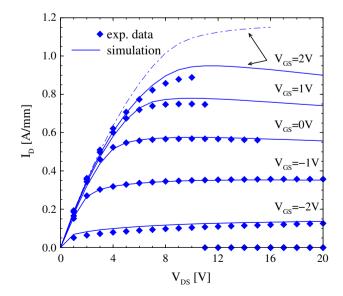


Fig. 8. Calibrated output characteristics versus experimental data for l_g = 0.25 μ m HEMT at 425 K. Dot-dashed line-w/o self-heating, solid line-with self-heating.

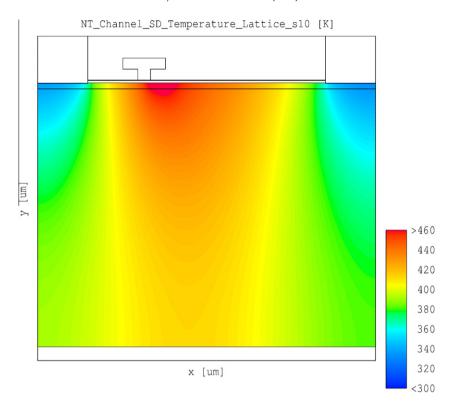


Fig. 9. Lattice temperature, calibration device, $V_{GS} = 2 \text{ V}$, $V_{DS} = 20 \text{ V}$.

while it maintains low calculation complexity and a good convergence behavior at the other hand. An extension accounting for three valleys is possible, was however ruled out due to the downgraded convergence.

3. Simulated devices

The epitaxial structures used in this work were grown by metalorganic chemical vapor deposition (MOCVD) on 3-in. semi-insulating SiC substrates. The layers consist of a highly-resistive c-plane GaN buffer, followed by a 22 nm thick Al_{0.22}Ga_{0.78}N barrier and finally a 3 nm thin GaN cap layer (Fig. 6). Room temperature Hall measurements on the 2DEG formed at the buffer to barrier interface resulted in a sheet carrier concentration of $8\times10^{12}\,\text{cm}^{-2}$ and a mobility of $1600\,\text{cm}^2/\text{Vs}$. After epitaxial growth, ohmic contacts were formed, showing a low contact resistance of $0.2\,\Omega$ mm. The nitride-assisted T-gate was used with two different gate lengths of $0.5\,\mu\text{m}$ and $0.25\,\mu\text{m}$, and was defined by e-beam lithography. The gate width W_g = $2\times50\,\mu\text{m}$ is taken as $1\times100\,\mu\text{m}$ in the simulation.

4. Simulation results

The $l_{\rm g}$ = 0.25 μ m structure serves as a calibration device. Based on the transfer characteristics we determine the already mentioned values for the interface charges. Using the same set of models and model parameters the $l_{\rm g}$ = 0.5 μ m benchmark device is simulated. The ambient temperatures at which the devices were measured and are simulated are 300 K, 365 K, and 425 K. For the gate-variation study, two more devices with $l_{\rm g}$ = 0.1 μ m and $l_{\rm g}$ = 0.15 μ m are simulated. Also a fourth ambient temperature of 485 K is explored.

4.1. DC results

Using the interface charges from Section 2.2 a very good agreement between measurement data and simulation results for the transfer characteristics of the calibration device ($l_{\rm g}$ = 0.25 µm) is achieved (Fig. 7). Our setup allows for a proper modeling of the drain current also at elevated temperatures. As an example, Fig. 8 shows the output characteristics at 425 K. Two curves are shown for $V_{\rm GS}$ = 2 V: without self-heating, which greatly overestimates the current; with self-heating, which delivers a significantly better match, but requires a higher computational effort.

While others [60] have observed a significant threshold voltage $(V_{\rm th})$ shift, in our measurements such is almost non-existent. As $V_{\rm th}$ depends on the carrier density, carrier trap density and the Schottky barrier height [61] we can assume that trapping effects in the devices are also temperature-independent in this range (the carrier density change is also negligible).

Fig. 9 shows the lattice temperature in the device ($V_{\rm DS}$ = 20 V, $V_{\rm GS}$ = 2 V bias). The area where the lattice is heated from high-energy electrons is the high-electric field region under the drain side of the gate and the gate-extension.

The same simulations are performed for the benchmark device ($l_{\rm g}$ = 0.5 μ m) next. Retaining the same interface charge values, a good prediction of the threshold voltage is obtained (Fig. 10). Raising the ambient temperature, once again yields a good agreement between simulation results and experimental data, also for the output characteristics (shown at 425 K in Fig. 11).

4.2. RF results

The RF device performance is studied by small-signal AC analysis [62]. Fig. 12 shows the current gain $|h_{21}|$ for the 0.25 μ m device for the three temperatures. The gain decreases at higher

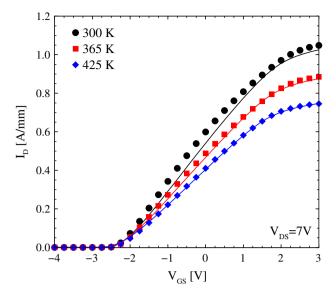


Fig. 10. Predicted transfer characteristics (lines) compared to measured data (symbols) for $l_{\rm g}$ = 0.5 μ m HEMT.

temperatures and the simulation agrees well with the measurements. The calculated cut-off frequency f_T is compared to the measured in Fig. 13. In order to account for the parasitics introduced by the measurement equipment the intrinsic parameters delivered by the simulation are transformed into extrinsic ones by using a standard two-port pad parasitic equivalent circuit. The values of the circuit elements are: $L_S=1$ pH, $L_G=44$ pH, $L_D=46$ pH, $C_{PGS}=36$ fF, $C_{PGD}=6$ fF, and $C_{PDS}=9$ fF. As mentioned in Section 3 the measured device has two gate fingers of 50 μ m width each, which leads to a higher gate capacitance due to three dimensional parasitic effects, than a single device with $W_g=100~\mu$ m as simulated.

We have achieved a very good agreement between measured and simulated S-parameters at all temperatures both for the calibration device ($l_{\rm g}$ = 0.25 μ m) and the benchmark device ($l_{\rm g}$ = 0.5 μ m). As an example, Fig. 14 compares the simulated and measured intrinsic S-parameters in the range 100 MHz–26 GHz

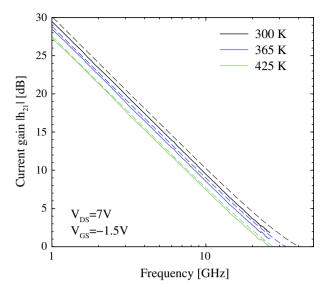


Fig. 12. Current gain $|h_{21}|$ for $I_g = 0.25 \, \mu m$ HEMT, experimental data (solid lines) versus simulation (dashed lines).

at $V_{\rm DS}$ = 7 V and $I_{\rm D}$ = 260 mA/mm for the $I_{\rm g}$ = 0.25 μ m HEMT at 300 K. Fig. 15 compares predictive simulation results for the $I_{\rm g}$ = 0.5 μ m device in the same frequency range, $V_{\rm DS}$ = 7 V, and $I_{\rm D}$ = 130 mA/mm at 425 K.

4.3. Gate length variation

Geometry of the transistors is pointed out to be an important factor for high-temperature operation. Consequently, several authors have studied the reduction of I_D with rising temperature for different gate lengths e.g. [8,57]. They agree, that for short channel devices ($I_g < 1 \ \mu m$) the carriers travel under the gate with saturation velocity. Therefore, the decrease of I_D is lower, as the decrease of the velocity in the saturation region is also lower. While we study only submicron devices, our results for $I_g = 1.0$ –0.25 μm structures agree well (Fig. 16) with those presented by Tan et al. However for very small gates an even lower temperature depen-

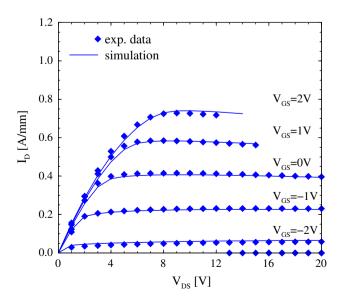


Fig. 11. Predicted output characteristics versus experimental data for l_{g} = 0.5 μm HEMT at 425 K.

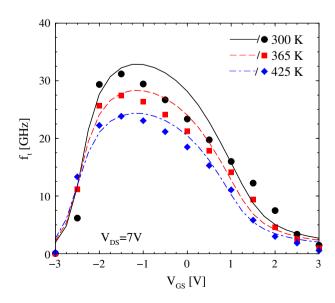


Fig. 13. Simulated cut-off frequency f_T (lines) compared to measurements (symbols) for l_g = 0.25 μm HEMT.

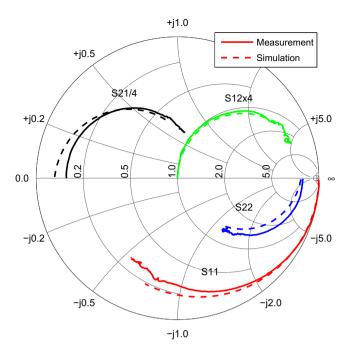


Fig. 14. S-parameters for the $l_{\rm g}$ = 0.25 μ m device at 300 K.

dence is observed. This same effect is more pronounced for the normalized f_T , where the l_g = 1.0–0.25 μ m devices deliver similar reduction of f_T with temperature, while the current gain cut-off frequencies of the sub-quartermicron devices decrease less (Fig. 17). We believe that for such gate lengths, not only l_g but also the gate-drain and gate-source distances and the exact geometry gain on importance, as for small gate lengths the parasitic contributions have to be scaled according to typical scaling rules in order to harvest the high-speed performance. In this case the relative contributions of the ohmic elements and thus their temperature dependencies are reduced.

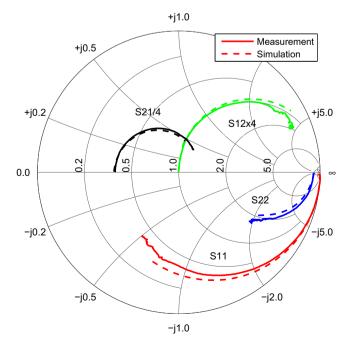


Fig. 15. S-parameters for the l_g = 0.5 μ m device at 425 K.

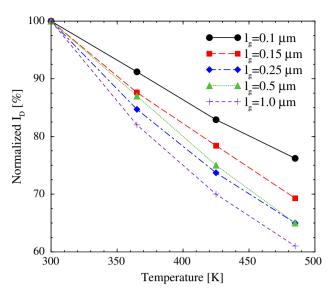


Fig. 16. Simulated maximum $I_{\rm D}$ ($V_{\rm DS}$ = 7 V) as a function of ambient temperature normalized to 300 K values.

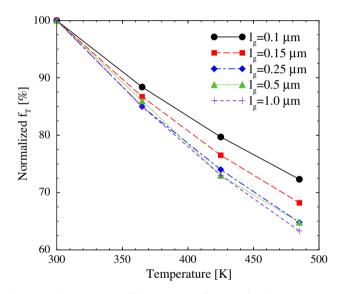


Fig. 17. Simulated maximum $f_T \left(V_{DS} = 7 \text{ V} \right)$ as a function of ambient temperature normalized to 300 K values.

5. Conclusion

A set of material and model parameters for hydrodynamic simulation of AlGaN/GaN HEMTs is presented. Relevant physical effects (such as self-heating) are accounted for. The set is validated against experimental data from a real device in a wide temperature range. Good predictive results for the DC and AC characteristics of another device are obtained. The calibrated simulation tool allows for the study, design and optimization of down-scaled structures for high-temperature operation.

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