Electron Mobility Models for III-Nitrides

Stanislay Vitanov and Vassil Palankovski

Abstract —In this work we present mobility models for electrons suitable for the drift-diffusion and the hydrodynamic transport models. The models describe specific effects, such as the negative differential mobility observed at high electric fields. The models are calibrated against Monte Carlo simulation results and experimental data for GaN, AlN, and InN. The models are suitable for implementation in simulation software tools. The models and the model parameters values are verified against measured transistor characteristics and allow simulation of various III-Nitride semiconductor devices.

 $\label{eq:Keywords-III-Nitrides, electron mobility, modeling, device simulation$

I. INTRODUCTION

Novel emerging devices based on the Nitride material system require physics-based models to properly describe their electrical and thermal behavior. Basic parameters for expressing the currents in a transistor are the carrier mobilities. While for Silicon well-established models exist [1], the III-V material system still poses certain challenges (e.g. the negative differential electron mobility at high electric fields applied) and is less studied in regard of novel materials, such as InN. Since the electrons are the main carrier type in modern III-V field effect transistors, such as HEMTs, we focus on the electron mobility in the following.

Several groups have proposed various models and model parameter sets for the simulation of GaN-based devices. Farahmand et al. [2] provide a low-field model which accounts for temperature and ionized impurity concentrations as well as a high-field model based on Monte Carlo (MC) simulation results. Another low-field model, valid in a large temperature and concentration range is proposed by Mnatsakanov et al. [3]. A highly parameterized field-dependent model based on an extensive data pool is developed by Schwierz [4]. Turin et al. [5] propose a high-field model which delivers excellent agreement with results from MC simulations. All these models are suited only for the drift-diffusion (DD) transport model. However, the latter is not able to deliver accurate results for sub-micron devices [6]. Therefore, the hydrodynamic (HD) transport model must be used for simulation of such devices. HD mobility models are needed, which not only describe well the electron transport properties under various conditions (temperature, density of defects and impurities, electric field, etc.), but are also easy to implement in a device simulator and are numerically stable. In this work we propose a consistent set (HD and DD) of such models.

S. Vitanov and V. Palankovski are with the Advanced Material and Device Analysis Group, Institute for Microelectronics, TU Wien, Gusshausstrasse 27/29, 1040 Vienna, Austria, e-mails: vitanov@iue.tuwien.ac.at, palankovski@iue.tuwien.ac.at

II. LOW-FIELD MOBILITY MODEL

The low field-electron mobility depends on lattice thermal vibrations, concentration of impurities, etc. The expression is independent of the transport model used.

$$\mu^{LI} = \mu^{\min} + \frac{\mu^{L} - \mu^{\min}}{1 + \left(\frac{C_{1}}{C^{\text{ref}}}\right)^{\gamma_{0}}}, \text{ where}$$

$$\mu^{L} = \mu^{L}_{300} \left(\frac{T_{L}}{300\text{K}}\right)^{\gamma_{1}}, \quad \mu^{\min} = \mu^{\min}_{300} \left(\frac{T_{L}}{300\text{K}}\right)^{\gamma_{2}}$$

 μ^{L} is the electron mobility in undoped material, μ^{min} is the mobility at highest doping, γ^{0} models the mobility decay with rising impurity concentration $C_{\rm I}$. γ^{1} and γ^{2} are used to model the dependence on the lattice temperature T_{L} . The model parameter values are summarized in Table 1.

TABLE 1. PARAMETER VALUES FOR THE LOW-FIELD MODEL

	Unit	GaN	AlN	InN
μ^{L}_{300}	[cm ² /Vs]	1600	683	10200
μ^{\min}_{300}	[cm ² /Vs]	100	29	500
C^{ref}	[cm ⁻³]	3×10 ¹⁷	5×10 ¹⁷	3.4×10 ¹⁷
γ^0		0.7	0.8	0.65
γ^1		-1.5	-3.21	-3.7
γ^2		-0.2	1.21	2.39

III. HIGH-FIELD MODELS FOR DD TRANSPORT

The models proposed for the high-field mobility are based on the mobility expression of the form [7, 8]:

$$\mu^{\text{LIF}}\left(E\right) = \frac{\mu^{\text{LI}}}{\xi + \left(\left(1 - \xi\right)^{\beta} + \left(\frac{\mu^{\text{LI}}E}{v^{\text{sat}}}\right)^{\beta}\right)^{1/\beta}} \tag{1}$$

 μ^{LI} is the low-field electron mobility as calculated previously, ν^{sat} is the saturated electron velocity, E is the electric field.

For the DD high-field mobility two different models are available. The first is the convenient model used for Silicon, referred as Model A. The second one is a modified model which accounts for negative differential mobility, referred as Model B. The latter is especially tailored to describe the transport properties of electrons in Nitrides. Further, based on Model B a corresponding HD model is synthesized.

A. Model A

The saturation velocity $v_{\rm sat}$ can be calculated in a separate model, accounting for its temperature dependence [book]. The parameter β models the slope of the mobility increase with increasing electric field, respectively electron driving force. While in the DD model it can be varied, a corresponding HD model can be obtained only for certain values. The model is derived from (1), with ξ =1/2. It offers excellent convergence behavior and a straight-forward calibration method. However, it cannot account for the velocity decrease at higher electric fields. Yet it offers a good agreement with the experimental data and MC simulation results for electric fields below the maximum velocity for all three materials (Fig. 1, Fig. 2, and Fig. 3) using the parameter setup provided in Table 2.

Table 2. Parameters for DD Model A

	Unit	GaN	AlN	InN
V _{sat}	[cm/s]	3×10 ⁷	3.7×10^7	5×10 ⁷
β		1.0	0.45	1.3

B. Model B

The model is based on the same expression for the electron mobility (1), with β =1 and ξ =1/2. In order to approximate the mobility decay due inter-valley transfer at high fields, two sets of μ are used. One describes the mobility $\mu_{\Gamma}(E)$ in the lower valley and the other one in the higher $\mu_{U}(E)$ (while Γ and U are the lowest two valleys only in GaN, this notation is retained for the other materials for simplicity):

$$\mu_{\Gamma}\left(E\right) = \frac{\mu_{\Gamma}^{LI}}{1 + \left(\frac{\mu_{\Gamma}^{LI}E}{v_{\Gamma}^{sat}}\right)}, \quad \mu_{U}\left(E\right) = \frac{\mu_{U}^{LI}}{1 + \left(\frac{\mu_{U}^{LI}E}{v_{U}^{sat}}\right)}$$

A weighted mean is built:

$$\mu^{\text{LIF}}\left(E\right) = \frac{\mu_{\Gamma}\left(E\right) + \mu_{\text{U}}\left(E\right)P_{\text{DD}}\left(E\right)}{1 + P_{\text{DD}}\left(E\right)}$$

where $P_{DD}(E)$ is the valley occupancy [9]:

$$P_{\rm DD}(E) = 6 \cdot \left(\frac{{\rm m_U^*}}{{\rm m_\Gamma^*}}\right)^{\frac{3}{2}} \exp\left(-\frac{\Delta E_{\rm C}}{kT_{\rm L} + \left(1 + E/E_{\rm 0}\right)}\right)$$

 m^*_{Γ} and m^*_{U} are the effective electron masses in the Γ and U valleys, respectively, ΔE_C is the difference in the conduction bands, and k is the Boltzman's constant.

This model allows setting a lower electron mobility and velocity in the higher conduction band. Thus, the decrease of the electron velocity at high electric fields, characteristic for most Nitrides can be well described.

Since all MC simulations and experiments, on which we rely to calibrate the low-field mobility in GaN, were performed at low electric fields, we set $\mu_{\Gamma} = \mu^{LI}$ as calculated

by the low-field mobility model. Using a down-scaled mobility ($\mu_U = 0.1 \times \mu^{LI}$ supported by MC data) and velocity in the higher band results in a decrease of the electron velocity at higher fields. Using the parameters listed in Table 3, the model delivers an acceptable approximation in comparison to MC simulations, accounting for as much as six bands [11] (Fig. 1). Results from different groups (see [12] and the references therein) vary widely (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 DD mobility model (and the corresponding HD model) are a carefully chosen trade-off. On the one hand they provide a velocity-field characteristics close to the one obtained by MC simulation, while on the other hand they maintain low calculation complexity and a good convergence behavior. An extension accounting for three valleys is possible, however, it was ruled out due to the downgraded convergence.

For AlN, the model cannot be applied due to the very slow increase of the velocity versus electric field. The simpler model A gives sufficiently good agreement (see Fig. 2).

Based on the recent MC simulation studies for InN accounting for the re-evaluated band gap (see [13] and the references therein), a parameter setup is extracted (Table 3). Due to the value of β close to 1, a good agreement can be achieved (Fig. 3) for velocity characteristics below the maximum, while a low value of E_0 accounts for the intervalley transfer at fields starting at 50 kV/cm.

Table 3. Parameters for DD Model B

	Unit	GaN	InN
$v_{\text{sat},\Gamma}$	[cm/s]	3×10 ⁷	6×10 ⁷
v _{sat,U}	[cm/s]	1×10 ⁷	1×10 ⁷
μ_Γ/μ^{LI}		1.0	1.0
μ_U/μ^{LI}		0.1	0.1
m^*_{Γ}/m^*_{0}		0.2	0.25
m^*_U/m^*_0		0.3	0.04
E ₀	[V/m]	0.26	0.035
ΔE_{C}	[eV]	1.4	1.78

IV. HIGH-FIELD MODELS FOR HD TRANSPORT

In order to obtain a consistent hydrodynamic mobility expression, the local energy balance equation:

$$E^2 \mu^{\text{LIF}} = \frac{3k(T_n - T_L)}{2q\tau_{\varepsilon}}$$

is solved for $E(T_n)$, which is then inserted into (1). This is performed again with $\xi=1/2$ for both models, and with $\beta=2$ for the first model and $\beta=1$ for the second model, respectively. T_n is the electron temperature and τ_e is the energy relaxation time.

A Model A

The expression obtained with the chosen values for ξ and β is identical with the one proposed by Hänsch et al. [8]. In order to account for NDM effects it is modified by introducing two parameters (γ_4 and γ_5):

$$\mu^{\rm LIT} = \frac{\mu^{\rm LI} \left(T_n / T_L\right)^{\gamma 4}}{\left(1 + \alpha^{1/\gamma 5}\right)^{\gamma 5}} \text{, where } \alpha = \frac{3k \mu^{\rm LI} \left(T_n - T_L\right)}{2q \tau_\varepsilon v_{\rm f}^2}$$

In the standard Hänsch model v_f corresponds to the saturation velocity v_{sat} (as in (1)). However, due to the powered temperature term $(T_n/T_L)^{\gamma 4}$ in the numerator the velocity is steadily decreasing at high-fields. Hence, v_f does not describe the saturation velocity as a physical quantity, although it does affect the high-field transport characteristics. The parameter γ_{5} has a more pronounced effect at low fields, while γ_4 influences primarily the highfield mobility, though their impact cannot be isolated to a specific field region. The conventional Hänsch model corresponds to the parameter set $\gamma_4 = 0$, $\gamma_5 = 1$. However, in order to approximate the simulation and experimental data, a set with $\gamma_4 = -0.3$ and $\gamma_5 = 2.4$ is chosen for GaN (Table 4). It delivers good agreement with the velocity-field characteristics obtained using the DD Model B (Fig. 1). Similar good match with DD Model A can be achieved also for AlN (Fig. 2). Only for InN it is not possible to model the very strong NDM effect.

TABLE 4. PARAMETERS FOR HD MODEL A

	Hänsch	GaN	AlN
γ ₄	0.0	-0.3	0.0
γ ₅	1.0	2.4	3.3

B. Model B

Inserting (6) into (1) with ξ =1/2 and β =2 gives the following expression for the high-field mobility. In order to approximate the inter-valley transfer at high fields, two sets of $\mu(T_n)$ are computed as in DD Model B.

$$\begin{split} \mu_{\Gamma} &= \frac{2\mu_{\Gamma}^{\mathrm{LI}}}{2 + \alpha_{\Gamma} + \sqrt{\alpha_{\Gamma}(4 + \alpha_{\Gamma})}}, \ \alpha_{\Gamma} = \frac{3k\mu_{\Gamma}^{\mathrm{LI}}(T_{n} - T_{L})}{2q\tau_{\varepsilon\Gamma}v_{\mathrm{f}}^{2}} \\ \mu_{\mathrm{U}} &= \frac{2\mu_{\mathrm{U}}^{\mathrm{LI}}}{2 + \alpha_{\mathrm{U}} + \sqrt{\alpha_{\mathrm{U}}(4 + \alpha_{\mathrm{U}})}}, \ \alpha_{\mathrm{U}} = \frac{3k\mu_{\mathrm{U}}^{\mathrm{LI}}(T_{n} - T_{L})}{2q\tau_{\varepsilon\mathrm{U}}v_{\mathrm{f}}^{2}} \end{split}$$

The weighted mean is built:

$$\mu^{\text{LIT}}\left(T_{n}\right) = \frac{\mu_{\Gamma}\left(T_{n}\right) + \mu_{\text{U}}\left(T_{n}\right)P_{\text{HD}}\left(T_{n}\right)}{1 + P_{\text{UD}}\left(T_{n}\right)}$$

The expression for P_{HD} is analogous to that for P_{DD}:

$$P_{\text{HD}}(T_n) = 6 \cdot \left(\frac{m_{\text{U}}^*}{m_{\text{F}}^*}\right)^{\frac{3}{2}} \exp\left(-\frac{\Delta E_{\text{C}}}{kT_n}\right)$$

TABLE 5. PARAMETERS FOR HD MODEL B

	Unit	GaN	InN
$ au_{\Gamma}$	[ps]	1.68	0.21
$ au_{ m U}$	[ps]	0.21	0.021

Fig. 4 compares the valley occupancy in GaN as a function of the electric field as calculated in this model and in MC simulation. The used parameter setup is the same as for DD Model B (Table 4). The only additional values needed, are the scaled energy relaxation times in the upper valley (Table 5). An excellent agreement between all models is achieved both for GaN (Fig. 1) and InN (Fig. 3), where the abrupt decay is reproduced very well. While the models deliver consistent results, the two approaches expose some differences. HD Model A is close to already established models and offers a straightforward calibration with only two auxiliary parameters (within a narrow value range). HD Model B is more complex, however, it allows for a more flexible calibration. Its parameters are derived from physical quantities.

Our models are calibrated against Monte Carlo simulation results and experimental data. They are implemented in our two-dimensional device simulator Minimos-NT (http://www.iue.tuwien.ac.at/mmnt) and are a part of model set, which provides excellent agreement with experimental data for various Nitride transistors at various conditions, e.g. see recent results in [14].

V. CONCLUSION

We present mobility models suitable for the drift-diffusion and hydrodynamic transport models for GaN, AlN, and InN. They provide a very good agreement with theoretical results and experimental data. Special attention is paid to the negative differential mobility phenomenon. The HD and the DD models deliver consistent results.

VI. ACKNOWLEDGEMENTS

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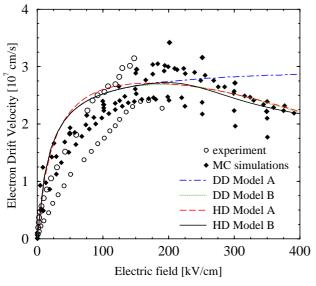


Fig. 1: GaN electron drift velocity versus electric field: simulations with different mobility models compared to MC simulation results and experimental data.

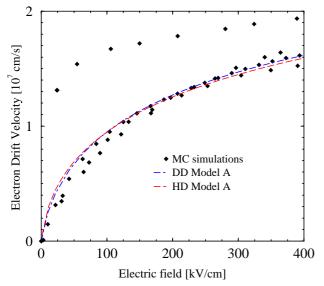


Fig. 2: AlN electron drift velocity versus electric field: simulations with different mobility models compared to MC simulation results.

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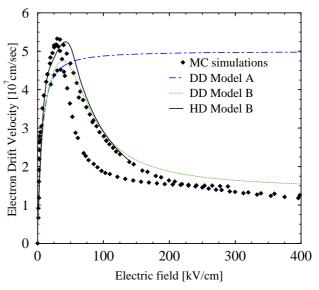


Fig. 3: InN electron drift velocity versus electric field: simulations with different mobility models compared to MC simulation results.

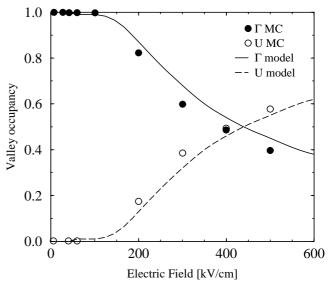


Fig. 4: GaN valley occupancy as a function of the electric field: model B versus MC simulation result.

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