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A temperature dependent model for the saturation velocity in semiconductor materials

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Abstract

Precise modeling of the saturation velocity is a key element for device simulation, especially for advanced devices such as e.g. High Electron Mobility Transistors (HEMTs) where the saturation velocity v_{sat} is directly related to the available gain of the device. We present a model implementing the temperature dependence of the saturation velocity v_{sat} into the two-dimensional device simulator MINIMOS-NT. The new model covers all relevant materials such as the elementary semiconductors Si and Ge, and the binary III-V group semiconductors GaAs, AlAs, InAs, GaP and InP. Furthermore, a composition dependent modeling for alloyed semiconductors such as e.g. $Si_{1-x}Ge_x$, $Al_xGa_{1-x}As$ or $In_xGa_{1-x}As$ is included. The implementation reflects a comprehensive literature survey on available experimental data and Monte Carlo (MC) simulation data. The work is completed by new MC simulations, especially for material compositions, where no experimental data are available. The extraction of the saturation velocity reveals a significant difference between the saturation velocity in the bulk and the effective (saturation) velocity extracted from rf-measurements e.g. for High Electron Mobility Transistors. Since this effective value is often used for device characterization, the difference gives insight into modeling the determining quantities of HEMTs.

Keywords: Saturation velocity; Modeling; Temperature; Device simulation

1. Introduction

State-of-the-art simulation requires precise modeling and fast computation. For the description of effects such as self-heating for a great variety of materials it is necessary to obtain universal models, that are suitable for all technologically relevant materials and keep the connection to physical quantities. Various models have been suggested for modeling the temperature dependence of the saturation velocity, see e.g. Mohammad [1], Allam and Pribetich [2]. Yet the models presented have either been restricted to a limited number of materials, seem to be unnecessarily complex in their mathematical form, or are not physically sound. The model suggested in this work covers all technologically relevant semiconductor materials over a wide temperature range of 200–400 K in a simple mathematical way.

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2. The saturation velocity for device simulation

Due to the high electric field in submicron devices, the saturation velocity plays an important role. Yet, several definitions appear about the term itself with respect to devices. In the simplified analytical device models, supplied e.g. by Delagebeaudeuf and Linh [3], the term "effective velocity" used in this context accounts for a lot of averaging processes. Particularly this averaging of the "effective" velocity includes:

1. the field dependence of the drift velocity;
2. intervalley transitions, where each valley has its own saturation velocity;
3. in quantum wells in e.g. HEMTs, two dimensional effects in the channel and interactions with neighboring materials.

It is questionable, whether the term "saturated" applies at all in this context, due to the averaging process also for non-saturated electrons. This is mentioned here, since in a number of publications Xu et al. [4], Dickmann et al. [5], Nguyen et al. [6] values from this concept of the saturation velocity in devices are extracted, that differ significantly from those extracted for the respective bulk materials. Our intention is not to question these values, but to reveal the difference between v_{sat} and $v_{(\mathrm{sat})\,\mathrm{eff}}$.

For the experimental and MC based extraction of the saturation velocity, the velocity above a certain electric field should not change within a certain accuracy, i.e. there exists a stable mean value of the saturation velocities in the different valleys in k-space. Yet, MC simulations e.g. in AlGaAs by Brennan et al. [7] suggest no saturation within the E-field range up to 400 kV/cm. To keep a concept of a saturated velocity for device simulation two conditions are given: the electric field, from which the saturated velocity is extracted, has to be high in comparison to the field prevailing in the major part of the device, and the regions where this high field actually applies, have to be relatively small. Since an electric field of about 100 kV/cm is accessible to measurement, values above that field shall be considered. For a device simulator such as MINIMOS-NT the functional form of mobility modeling is particularly important, see Selberherr [8]. The high field mobility for the hydrodynamic simulation is modeled according to Hänsch et al. [9]:

$$\mu = \frac{\mu^{\mathrm{LIS}}}{1 + \alpha \cdot (T - T_{\mathrm{L}})} \tag{1a}$$

$$\alpha = \frac{3 \cdot k_B \cdot \mu^{\mathrm{LIS}}}{2 \cdot q \cdot \tau \cdot v_{\mathrm{sat}}^2} \tag{1b}$$

μ^{LIS} represents the lattice mobility and also considers impurity and surface scattering, T is the carrier temperature and τ(E) the field dependent energy relaxation time. It has to be stated that the device simulator uses one-valley models for most of the quantities, many valley properties of semiconductors are modeled by effective values. As stated by Selberherr [8], a doping dependent modeling of the saturation velocity is not considered to be reasonable. Experimental results, see e.g. Sabnis and Clemens [10], prove the assumption that the doping does not influence the saturation velocity. An important factor is the influence of the electric field orthogonal to the velocity. Additionally the crystal orientation has an influence on the saturation velocity, e.g. in silicon, see Canali et al. [11].

3. The model

The model used in MINIMOS-NT is based on formula (2):

$$v_{\mathrm{sat}}(T_{\mathrm{L}}) = \frac{v_{\mathrm{sat300}}}{(1 - A) + A \cdot (T_{\mathrm{L}}/300)} \tag{2}$$

The model is a two parameter model, where the first parameter, v_{sat300}, represents the saturation velocity at the lattice temperature $T_{\mathrm{L}} = 300$ K. The second parameter, the temperature coefficient A, reflects the temperature dependence of the various materials covered by the model.

For a material of A_xB_{1-x} the saturation velocity is interpolated in the following way:

$$\begin{aligned} v_{\mathrm{satAB}} = {} & x \cdot v_{\mathrm{satA}}(T_{\mathrm{L}}) + (1 - x) \cdot v_{\mathrm{satB}}(T_{\mathrm{L}}) \\ & + x \cdot (1 - x) \cdot v_{\mathrm{satbowAB}} \end{aligned} \tag{3}$$

The bowing parameter v_{satbowAB} is introduced to account for a nonlinear bowing prevailing in some materials. The errors of analytical fitting are found to be insignificant relative to the uncertainties of the measured data.

4. Monte Carlo simulations

For the bowing parameter v_{satbowAB} and for investigation of holes in GaAs the available data were supplemented with MC simulations. The standard particle model, see Moglestue [12], was used. To calculate the bulk drift velocity we dispense with the Poisson part and instead impose a constant electric field and only update the wave vector or velocity of the individual particles at the end of their free flights. The steady state average drift velocity is obtained from an ensemble of 2000–6000 particles over an interval of 10 ps. The only material parameters needed are the effective

mass in the three minima of the Brillouin zone, the acoustic deformation potential, the static and optical frequency dielectric constants, energy of the phonons causing transfer between the various minima of the Brillouin zone and the band gaps. Ionized impurity scattering is included in the model but found to be of no significance at the chosen electric field (100 kV/cm) and donor concentration (10^{15} cm^{-3}). Neutral impurity and interparticle scattering have been excluded from the model because they are of minor importance. Nor has alloy scattering been considered because it depends on the ordering of the cations in the lattice, which depends on the history of the crystal growth so that a comparison with experimental data would require knowledge of the ordering. The bulk drift velocity in the pure III-V compounds and alloys have been calculated by the same method used by several authors e.g. Brennan and Hess [13], however, there are less experimental data than calculated ones. We have adjusted our parameters to best fit available experimental data.

For the alloy A_xB_{1-x} we take the material parameter p, to be:

$$P_{AB} = x\,P_A + (1-x)\,P_B + x\,(1-x)\,b \tag{4}$$

where b represents a bowing parameter which we have taken to be zero except for the values of the energy difference between the minima in the conduction band, which we have used the values quoted by Krijn [14]. For bulk alloys very few experimental values are available. The same set of material parameters also applies to holes. Only the Luttinger [15] parameters can be adjusted to get the respective bulk hole velocity.

Table 1
Model parameters for formulas (2–3)

Material	A (−)	v_{sat300} (10^7 cm/s)	$v_{satbowAB}$ (10^7 cm/s)
Si electrons	0.74	1.02	–
Si holes	0.37	0.72	–
Ge electrons	0.45	0.70	–
Ge holes	0.39	0.63	–
$Si_{1-x}Ge_x$ electrons	–	–	−2.28
$Si_{1-x}Ge_x$ holes	–	–	0[a]
GaAs electrons	0.44	0.72	–
AlAs electrons	0.45	0.85	–
InAs electrons	0.43	0.9[b]	–
$Al_xGa_{1-x}As$ electrons	–	–	−0.051
$In_xGa_{1-x}As$ electrons	–	–	−0.196
$In_xAl_{1-x}As$ electrons	–	–	−2.13
GaAs holes	0.59	0.9	–
$In_{0.53}Ga_{0.47}As$ holes		0.48	–
GaP electrons	–	0.88	–
InP electrons	0.31	0.68	–
$In_{1-x}Ga_xP$ electrons	–	–	−0.3[b]
InP holes	–	0.7	–
$In_{0.48}Ga_{0.52}P$ holes	–	0.74	–

[a] See the strain dependence in Bufler et al. [22].
[b] Impact ionization is not included into the parameter.

5. Results

The collection of parameters is given in Table 1. Results obtained for electrons in silicon are shown in Fig. 1. Table 2 gives the sources of data used for Si and Ge for electrons and holes.

For electrons in $Si_{1-x}Ge_x$ the value for the bowing parameter was obtained from data given by Bufler et al. [22] as shown in Fig. 2 in the range of $x < 0.3$. A bowing parameter for holes in $Si_{1-x}Ge_x$ can be obtained from Yamada and Ferry [20] for MC simulation for E = 350 kV/cm. The values correlate strongly with the strain applied so no general bowing parameter is given here.

For GaAs electrons the values were obtained from the extrapolated values of Houston and Evans [23] to 120 kV/cm, which are in agreement with results obtained by Windhorn et al. [24] and references therein. For GaAs holes the experimental results available represent a relatively poor base for the temperature dependence. Many references can be traced back to Dalai et al. [25]. The values given by Dalai et al. [25] and Dalai [26] appear too high in comparison to GaAs electrons and to more plausible experimental values obtained by Holway et al. [27]. Our work supplies additionally new MC data for GaAs obtained at 100 kV/cm shown in Fig. 3.

Due to the transition to an indirect semiconductor the values for v_{sat} in $Al_xGa_{1-x}As$ were acquired for the range of $x < 0.4$ relevant for device simulation for the bowing. Fig. 4 shows our MC values obtained for AlGaAs. It has to be stated that the significant bowing due to the direct-indirect transition was not included into the bowing factor given in Table 1 for the sake of simplicity: the model of equation (3) cannot account

Table 2
Sources of data for Si and Ge

Material	Reference	Data
Electrons in Si	Jacoboni et al. [16]	Experiments
Holes in Si	Canali et al. [11]	Experiments
	Fischetti et al. [17]	MC simulation
Electrons in Ge	Jacoboni et al. [18]	Experiments
Holes in Ge	Reggiani et al. [19]	Experiments
	Yamada and Ferry [20]	MC simulation
	Fischetti [21]	MC simulation

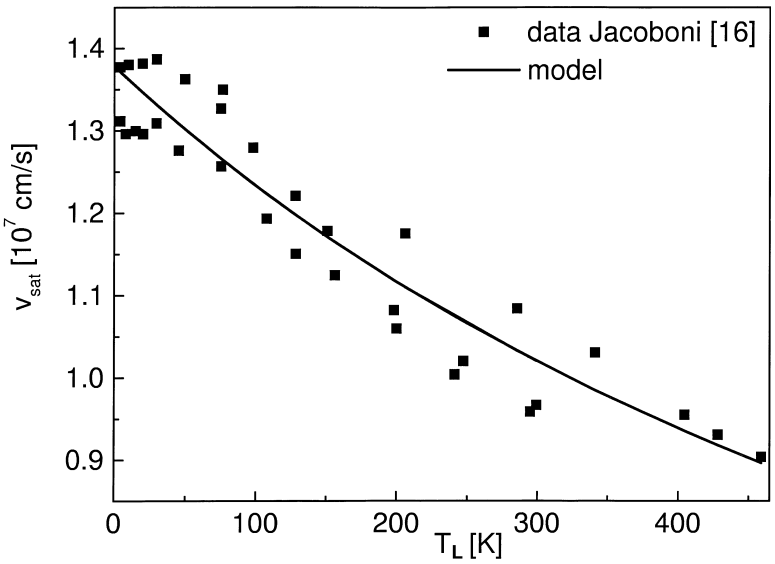

Fig. 1. Demonstration of the model for the v_{sat} data of electrons in silicon by Jacoboni [16].

for this bowing and at the same time supply accurate values for the range $x < 0.4$ relevant for device simulation.

For InAs we found, as also stated by Brennan and Hess [13] and Fischetti [21], that v_{sat} depends strongly on the degree of impact ionization assumed in the MC simulation due to the small bandgap. The results obtained without or with impact ionization differ from 0.9 to 8–12 $\times$ 10^7 cm/s. For this reason the bowing parameter and the values for $In_xGa_{1-x}As$ were not directly interpolated in equation (3) from InAs, but from the well investigated $In_xGa_{1-x}As$ for $x \leq 0.53$, see Windhorn et al. [28], Brennan and Park [29]. The bowing parameter and v_{sat} for InAs given are therefore only valid without impact ionization. If this effect is included into device simulation v_{sat} has to be adapted with respect to the modeling of the impact ionization. The temperature dependence of $In_xGa_{1-x}As$ results was obtained for $InGa_{0.53}As_{0.47}$ from our own MC simulation as shown in Fig. 5. It was found that the

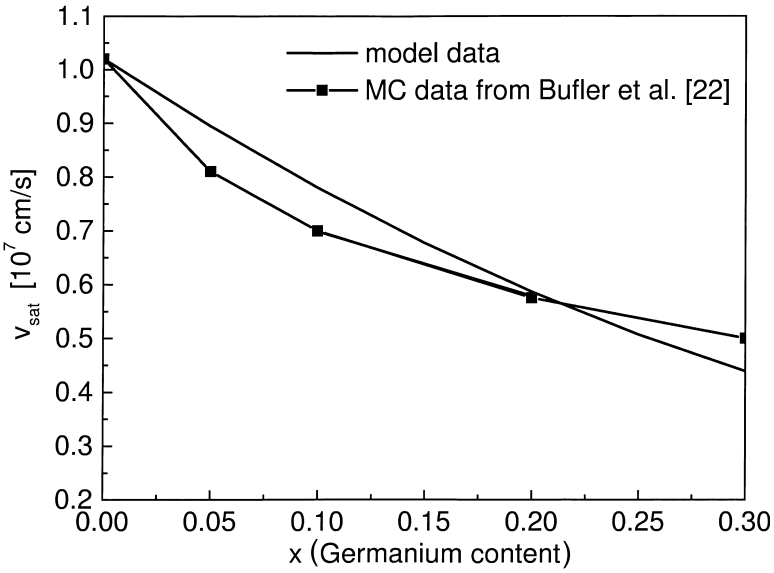

Fig. 2. Comparison of modeling the bowing for electrons in $Si_{1-x}Ge_x$ with data supplied by Bufler et al. [22] for $x < 0.3$.

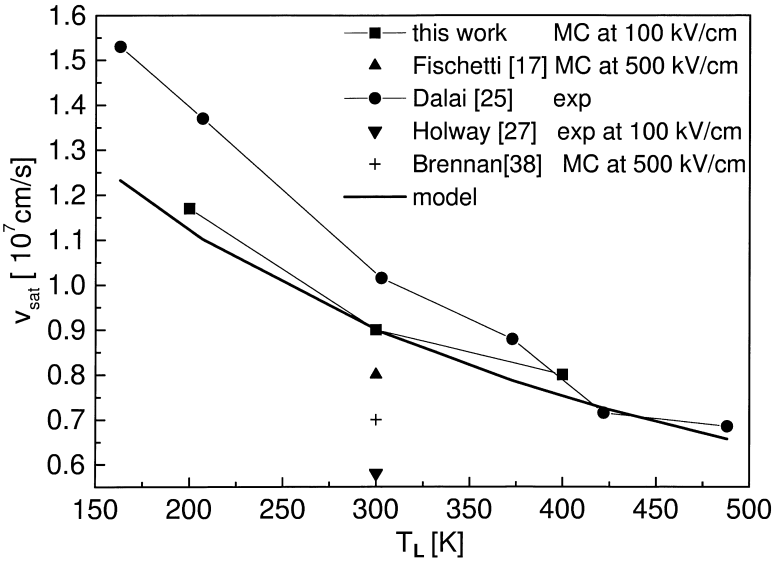

Fig. 3. Comparison of experimental, MC simulations, and the model for holes in GaAs.

assumption of temperature independent bowing is correct within the validity of the model.

For $In_xAl_{1-x}As$ the bowing parameter is similarly influenced by the impact ionization of InAs. The experimental basis is poor. The bowing parameter is obtained from Kim et al. [30] for $In_{0.52}Al_{0.48}As$ for $E = 35$ kV/cm at various temperatures. Our own MC simulations support this value for the bowing assuming no impact ionization.

The base for the extraction of v_{sat} of holes in AlGaAs was considered to be insufficient. For holes in n-type $In_{0.53}Ga_{0.47}As$ experimental data is found in Hill et al. [31], MC simulation data in Brennan [32].

The scatter of the values for electrons in InP, shown in Fig. 6 for 300 K, is not due to the influence of the electric field only. Temperature dependent values were obtained from Fischetti [21] and Windhorn et al. [33]. The latter values for 120 kV/cm are higher than found by Robson et al. [34] and Boers [35].

For electrons in GaP experimental values for $T_L = 300$ K are taken from Johnson et al. [36] and

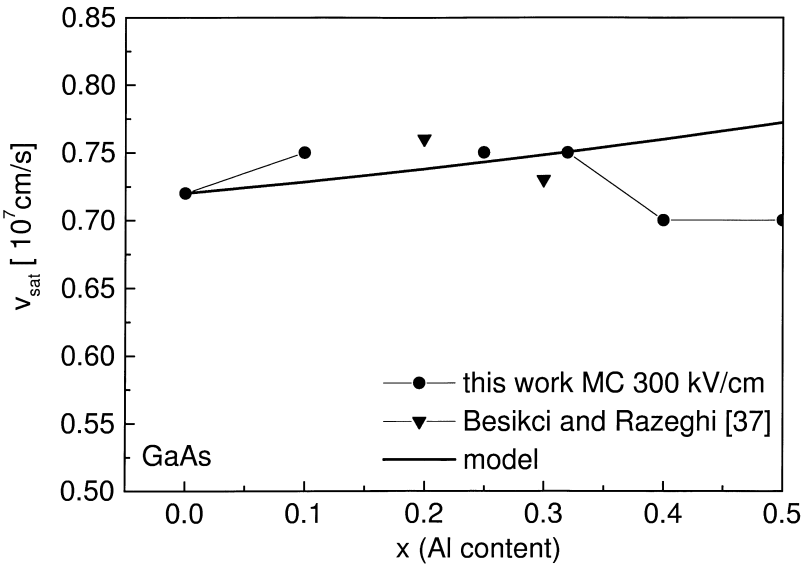

Fig. 4. Simplification of the bowing in $Al_xGa_{1-x}As$ for $x < 0.45$.

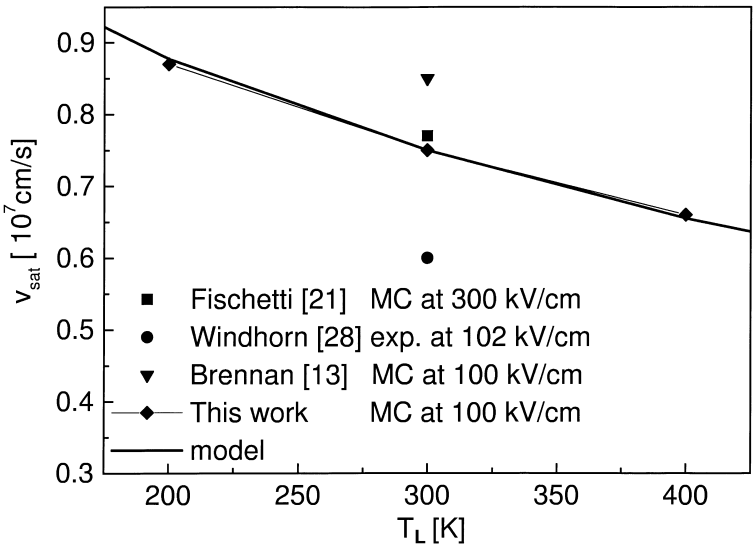

Fig. 5. Temperature dependence of v_{sat} in $In_{0.53}Ga_{0.47}As$.

from MC simulations by Fischetti [21]. For $In_{1-x}Ga_xP$ the bowing parameter was obtained at 400 kV/cm from Besikci and Razeghi [37]. The temperature dependence in GaP could not be determined, since we found no sufficient data base for $T_L \neq 300$ K.

For holes in InP MC simulation data is supplied by Brennan and Hess [38]. Further for $In_{0.48}Ga_{0.52}P$ data is given by MC simulations by Brennan and Chiang [39].

With respect to devices, the preceeding results reveal the difference of the effective velocities and the saturation velocities extracted here at electric fields above 100 kV/cm. Table 3 shows a comparison of the model values for v_{sat} and effective values $v_{sat\,eff}$ obtained from literature.

The results reveal the difference, since the effective values are significantly larger.

Since the model shall be applied to HBTs with a basically three-dimensional as well as for HEMTs with a basically two-dimensional structure, the modeling of the saturation velocity must be independent of this difference. Therefore the effects leading to such high values of $v_{sat\,eff}$ in HEMTs have to be modeled separately. These effects to be modeled are impact ioniz-

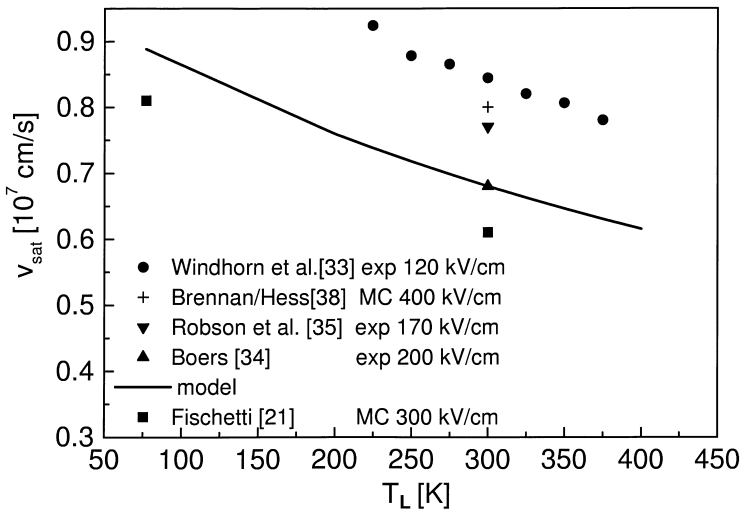

Fig. 6. Temperature dependence of the saturation velocity for electrons in InP.

Table 3
Comparison of the effective $v_{sat\,eff}$ in HEMTs and the modeled saturation velocity v_{sat}

Material	$v_{sat\,eff}$	Author	$v_{sat\,model}$
$Al_{0.22}Ga_{0.78}As/In_{0.05}Ga_{0.95}As$	1.59×10^7 cm/s	Dickmann et al. [5]	0.72×10^7 cm/s
$In_{0.20}Al_{0.80}As/In_{0.53}Ga_{0.47}As$	3.1×10^7 cm/s	Nguyen et al. [6]	0.75×10^7 cm/s

ation, the correlation of real space transfer and velocity overshoot, and the two-dimensional mobility in the channel.

6. Conclusion

We demonstrate a simple and precise model for the saturation velocity as a function of temperature in the range of 200–400 K for a large number of technologically relevant semiconductors with respect to the simulation of advanced Bipolar and Heterostructure Devices.

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