Electron Transport Properties of Gallium Nitride for Microscopic Power Device Modelling

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Abstract. The design of power GaN devices has to take into account the impact of temperature on device materials due to highly dissipated power and a consequent large self-heating. The accurate knowledge of transport properties as a function of the lattice temperature is essential in order to make a good thermal management to optimise the device performance. In this paper, accurate expressions describing the main transport properties as a function of the lattice temperature and electric field for wurtzite GaN have been extracted starting from Monte Carlo simulations and then using a genetic algorithm. In particular, these expressions take into account the abrupt change in electron velocity slope at a low electric field (∼20 kV/cm). Using the same methodology, we have determined the temperature dependence of other physical parameters such as the low field mobility, saturation velocity, critical electric field and the corresponding peak velocity in a temperature range of 300 K - 700 K. The results show a very good agreement between the theoretical and experimental values.

1. Introduction

Semiconductor devices based on III-Nitrides have been widely accepted as a good vehicle for high frequency and high power applications [1][2]. In particular, gallium nitride presents remarkable electrical and thermal properties such as a high bandgap (3.4 eV), a high saturation velocity ($v_{sat} > 1 \times 10^7 \text{cm/s}$) and a high breakdown electric field (3 MV/cm) associated to an excellent thermal conductivity (1.6 W/cm.K) [3][4].

III-Nitrides based devices can take the wider bias ranges without inducing breakdown of the device. At very high biases, a self-heating occurs in the device and considerably increases the lattice temperature which negatively affects transport properties [4][5]. Therefore, the simulation of such devices has to account for thermal effects in order to obtain more accurate results [6][7]. The numerical investigations of such devices need an accurate knowledge of the temperature dependence of the transport properties, mainly the carrier velocity.

In this paper, the transport properties of GaN are determined from bulk Monte Carlo data. Starting from Monte Carlo results and using Genetic Algorithm (GA), it is possible to extract an analytical function, which describes the electron drift velocity of wurtzite-GaN versus the lattice temperature and electric field. The GA is used to determine the lattice temperature dependence of other physical parameters such as the low field mobility, saturation velocity, critical electric field and the corresponding peak velocity.
2. Monte Carlo calculations

The transport properties of GaN are obtained from stationary Monte Carlo (MC) simulations for different lattice temperatures (in a range of 300 K - 700 K by step of 50 K) and for ionised impurity concentrations of $10^{15}/\text{cm}^3$ and $10^{17}/\text{cm}^3$, respectively [8]. The used MC code is based on a three isotropic and non parabolic valley model. The scattering mechanisms included in the simulations are optical acoustic phonons, piezoelectric, intervalley scattering and ionized impurities. The valley parameters are deduced from band structure calculations [9], and the coupling constants involved in scattering rates are taken from [10].

Figure 1 shows that the average drift velocity drops as the lattice temperature increases at a fixed electric field. This is due to the total scattering rate increasing as the lattice temperature increases [12]. Indeed, the higher temperature results in the increase of the phonon scattering rate due to a larger phonon occupation number [13]. The dominant scattering mechanisms, at low electric fields, are polar optical phonon absorption, an interaction with ionised impurities and acoustic phonon scattering. As the electric field increases, a substantial number of electrons get sufficient energy and consequently the polar optical phonon emission becomes possible. The slope of the electron velocity at low electric field decreases abruptly at approximately 20 kV/cm due to the onset of polar optical phonon emission [14]. However, this phenomenon vanishes at high temperatures. At high electric fields, close to 200 kV/cm, the electrons gain enough energy for a transfer into the satellite valleys by the intervalley phonon scattering and therefore a peak velocity is observed. In addition, this increased relaxation of electron energy and momentum results in a higher threshold electric field for heating of electrons. This increases their probability to scatter into the satellite valleys [15]. Thus, if we assume the constant separation energy for satellite valleys (we neglect a band gap renormalization due to the change in temperature), the threshold electric field increases with temperature while the peak velocity decreases. The Monte Carlo results show that the electron effective masses and the energy relaxation times are nearly identical for all considered lattice temperatures. Thus, mobility is the only quantity that strongly depends on lattice temperature.

3. Results and discussion

Starting from Monte Carlo data, the GA was implemented in order to determine a new expression of drift electron velocity for GaN versus electric field in respect to a temperature range of 300 K - 700 K:

$$V(E, T) = \frac{\mu_n(T) E + \frac{v_{0} + v_{sat}(T) [E/E_2(T)]}{1 + [E/E_2(T)]^4} [E/E_C(T)] \alpha}{1 + [E/E_C(T)]^4}$$

$$v_0 = \left[2v_{peak}(T) - \frac{\mu_n(T) E_C(T)}{1 + E_C(T)/E_3(T)} \left[1 + \left(E_C(T)/E_2(T)\right)^4\right] - v_{sat}(T) \left(E_C(T)/E_2(T)\right)^4\right]$$

where $T$ is the lattice temperature in Kelvin, $\mu_n$ is the low field mobility, $E_C$ is the critical electric field, $v_{peak}$ is the peak velocity and $v_{sat}$ is the saturation velocity. These parameters are determined as function of the temperatures. A good agreement is observed between Monte Carlo results and the analytical determinations for the two ionized impurity concentrations (figure 1).

Based on GA optimisation, the extracted analytical expressions describing the low field mobility $\mu_n[\text{cm}^2/\text{V.s}]$ as well as saturation $v_{sat}[\text{cm/s}]$ velocity at high electric fields and for two ionized impurity concentration as a function of the lattice temperature are:

| $N_D=10^{19}/\text{cm}^3$ | $N_D=10^{17}/\text{cm}^3$ |
|--------------------------|--------------------------|
| $\mu_n(T)$ | $634 - 204 \frac{T}{300} + 80.9 \times 10^3 \ exp\left(-4 \frac{T}{300}\right)$ | $120 + 4.9 \times 10^3 \ exp\left(-1.88 \frac{T}{300}\right)$ |
| $v_{sat}(T)$ | $2.05 \times 10^8 - 78.9 \times 10^4 T$ | $3.56 \times 10^8 - 17 \times 10^3 T$ |
Figure 1. Electron drift velocity versus electric field of GaN for different lattice temperatures (in a range of 300 K - 700 K by step of 50 K): (A) $N_D=10^{15}/\text{cm}^3$ and (B) $N_D=10^{17}/\text{cm}^3$. Monte Carlo data (dash line) are compared to the genetic algorithm results (solid line).

Figure 2 shows the measured and analytical determination of the low field mobility at $N_D=10^{15}/\text{cm}^3$ as well as comparison between the analytical determination and results obtained from Ref.[16] for $N_D=10^{17}/\text{cm}^3$. The electron mobility saturation is observed at very high temperature primarily limited by longitudinal optical (LO) phonon scattering. The measurements of low field mobility have been carried out in the temperature range of 300 K to 500 K using Hall effect. We observe the large drop of the electron mobility between $N_D=10^{15}/\text{cm}^3$ and $N_D=10^{17}/\text{cm}^3$. The theoretical predictions are compared to experimental results [16] observing a very good agreement.

Figure 2. Low field mobility of GaN versus lattice temperature. Measured (circles) and analytical determination (solid line) at $N_D=10^{15}/\text{cm}^3$ are compared to the analytical determination (dash line) and results of Ref. [16] (squares) at $N_D=10^{17}/\text{cm}^3$.

Figure 3. Saturation velocity of GaN versus lattice temperature for $N_D=10^{15}/\text{cm}^3$. Comparison between the results of Ref. [11] (dash line) and the GA expression (solid line).

Figure 3 show that the saturation velocity decreases significantly when the temperature increase. The velocity versus electric field evolution is due to the larger electron effective mass increase in the satellite valleys. A very good agreement is also observed for $N_D=10^{15}/\text{cm}^3$ when our results
are compared to results of Ref. [11].
For the critical electric field and the associated peak velocity, we have obtained the following expressions for the temperature dependence:

\[
N_D = 10^{15}/\text{cm}^3 \\
E_{\text{peak}}(T) = 135 \times 10^4 + 10^5 T \\
v_{\text{peak}}(T) = 3.6 \times 10^{-1} - 175.3 \times 10^2 T
\]

The drop in the peak velocity with temperature is less than those currently observed in other semiconductors such as GaAs [11]. When the lattice temperature varies from 300 K to 700 K, the associated electric field increases by about 25 % and the peak velocity decreases by about 23 % (figure 3).

In the 300 K - 700 K temperature range, the evolutions of the other parameters used in the drift velocity expression as a function of the temperature are given by the following equations:

\[
\begin{align*}
N_D & = 10^{17}/\text{cm}^3 \\
E_2(T) & = 9.3 \times 10^5 \left( \frac{T}{300} \right)^{0.1166} \\
E_3(T) & = 52.5 \times 10^2 \exp \left( 1.65 \left( \frac{T}{300} \right) - 150.2 \times 10^2 \right) \\
\alpha(T) & = 4.15 + 74.6 \times 10^{-3} \exp \left( 1.1 \left( \frac{T}{300} \right) \right)
\end{align*}
\]

4. Conclusion
In this paper, we have extracted an analytical expression describing the dependence of the electron velocity as function of lattice temperature and electric field. This extraction is carried out starting from Monte Carlo simulations and then using GA. The same methodology is used to determine the lattice temperature dependent of low field mobility, saturation velocity, critical electric field and the corresponding peak velocity. The obtained analytical expressions describe the main transport properties of GaN in a temperature range of 300 K - 700 K. In particular, these expressions take into account the abrupt change in the electron velocity at low electric field. The results show a very good agreement between the theoretical and experimental results. This accurate analytical determination is absolutely necessary for simulation of power GaN devices which need an accurate information about electron velocity. The temperature dependence of electron velocity must be taken into account due to the highly dissipated power and the consequent large device self-heating. This constitutes an essential tool for the prediction of thermal management in GaN based power devices.

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