# CALCULATION OF THE ELECTRON MOBILITY OF GaN SEMICONDUCTOR COMPOUND USING THE MONTE CARLO METHOD★

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*Received December 21, 2004*

The electron mobility of GaN semiconductor compound was calculated by using the Monte Carlo method. We considered polar optical phonon scattering, deformation-potential acoustic phonon scattering and impurity scattering mechanisms. We investigated temperature dependence of mobility and drift velocity dependence of mobility for the compound. We compared our results with the literature.

*Key words:* Monte Carlo, GaN, electron transport.

## 1. INTRODUCTION

A wide-gap semiconductor, GaN, has been studied intensively for high temperature electronics, ultraviolet detectors and blue electroluminescent devices. GaN is one of the best candidates among other wide-band-gap materials for optoelectronic and electronic applications [1]. The direct nature of its band gap makes GaN ideal for optical detection and emission within the ultraviolet portion of the electromagnetic spectrum. Furthermore, the large band gap results in a large breakdown field, makes GaN especially suitable for high-power and high-speed applications [2].

The study of the transport properties is therefore essential for improvement of an advanced GaN device technology. The steady-state electron velocity has been calculated by several authors using the Monte Carlo method. These calculations are made by assuming either one or two valley analytical band structure [3].

In this study, we present calculations of drift velocity, mobility, mean electron energy and valley occupancy versus applied field in bulk GaN zinc blende phase.

★ Paper presented at the 5th International Balkan Workshop on Applied Physics, 5–7 July 2004, Constanța, Romania.

## 2. MONTE CARLO SIMULATION

The Monte Carlo method is often used in novel device simulations. It provides a useful tool for the development, analysis, and understanding of semiconductor devices. The Monte Carlo method in which the Boltzmann equation is not directly solved, but the distribution function and the transport coefficients are evaluated by the simulation of electron trajectories using random numbers. The method has been applied in different forms to solve transport problems in various kinds of physical phenomena [4]. The single particle Monte Carlo method, as applied to charge transport in semiconductors, consists of a simulation of the motion of one electron inside the crystal, subject to the action of external forces due to applied electric field and of given scattering mechanisms. The motion of electron is determined by collisions and external forces. The effect of external forces is deterministic, but the collision processes affect the motion in a probabilistic manner [5]. The former effect may be calculated by applying the classical laws of motion, but the latter effect is required to be evaluated by applying the probability theory. The duration of the carrier free flight and the scattering events involved in the simulation are selected stochastically in accordance with some given distribution probabilities describing microscopic processes [6–8]. As a consequence, any Monte Carlo method relies on the generation of a sequence of random numbers with given distribution probabilities.

## 3. SIMULATION RESULTS

A two-valley model of the conduction band using parameters for zinc blende GaN is used. Nanparabolicity is considered in two valleys. The scattering mechanisms considered in the simulation are polar optical phonon, ionized impurity, acoustic phonon and intervalley scatterings. Monte Carlo simulation was performed for the two conduction band at different lattice temperatures. For the calculations a fixed ionized impurity concentration of $10^{17}$ cm$^{-3}$ was used. Material parameters have been taken from literature. Different lattice temperatures were considered in the simulations of the effect of the lattice temperature on the steady-state electron drift velocity-field relation in GaN. Drift velocity decreases with increasing lattice temperature due to the increased total scattering rate for the applied electric fields considered as shown in Fig. 1. Dominant scattering mechanisms for low electric field strength are ionized impurity, polar optical phonon and acoustic phonon scatterings. As the applied electric field increases electrons gain sufficient energy and the polar optical phonon scattering become dominant as shown in Fig. 2.

*Table 1*

GaN material parameters used for the calculation

| Parameter | Value | Ref. |
|---|---|---|
| Band-gap energy [eV] | 3.52 | [9] |
| Effective mass at Γ ($m_0$) | 0.22 | [10] |
| Static dielectric constant ($\varepsilon_s / \varepsilon_0$) | 10.4 | |
| Acoustic deformation potential [eV] | 9.2 | |
| Velocity of sound [m/s] | 6590 | [11] |
| Effective mass at L ($m_0$) | 0.40 | |
| High-frequency dielectric constant ($\varepsilon_\infty / \varepsilon_0$) | 5.47 | [12] |
| Optical phonon energy [meV] | 92 | [13] |
| Density [g/cm$^3$] | 6.1 | [14] |
| Γ-L Energy separation $\Delta E_{\Gamma-L}$ [eV] | 2.0 | |

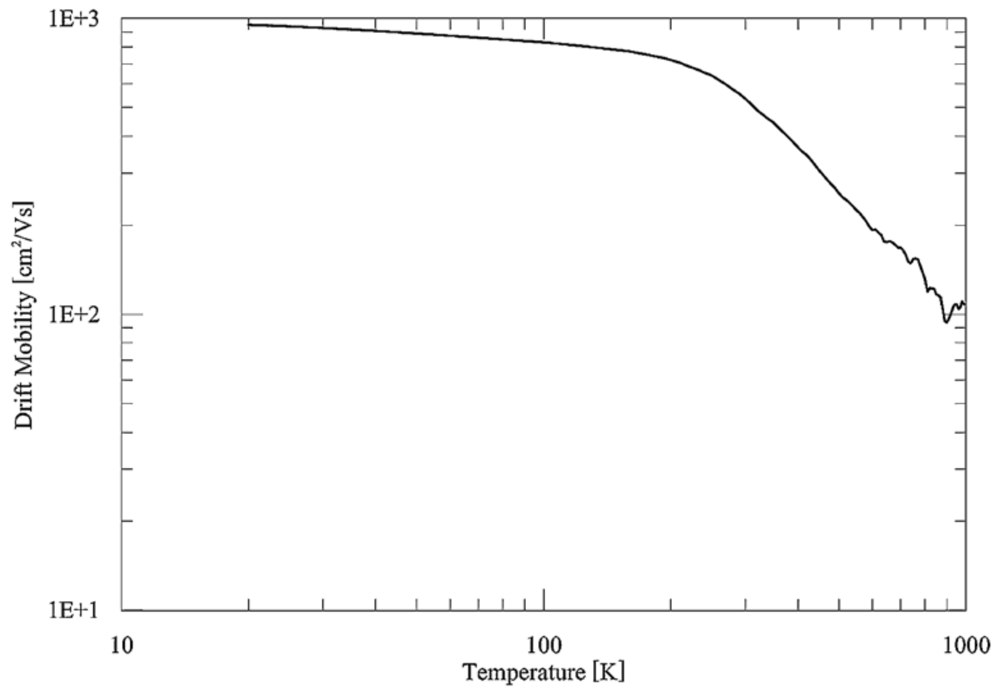


Fig. 3. – Electron mobility in GaN as a function of the lattice temperature at the $2 \times 10^6$ V/m electric field strength.

Drift velocity achieves $2.8 \times 10^5$ m/s maximum value in our simulation at $1.75 \times 10^7$ V/m for 300 K lattice temperature. It is reported in ref. [3] and ref. [9]

$3 \times 10^5$ m/s. As the applied electric field is further increased the drift velocity peaks starts to decrease.

Drift mobility was calculated as a function of the lattice temperatures for the constant electric field value of $2 \times 10^6$ V/m. Fig. 3 shows the electron mobility *versus* lattice temperatures.

## 4. CONCLUSION

We have performed single Monte Carlo simulations of the velocity-field and drift mobility-lattice temperature characteristics of zinc blende GaN. The simulations have included the nanparabolicity. The scattering mechanisms considered were polar optical phonon, acoustic phonon, intervalley and ionized impurity scatterings. Effects of the scatterings mechanisms on the drift velocity and mobility were analyzed. It was shown that polar optical phonon scatterings play an important role on the drift velocity.

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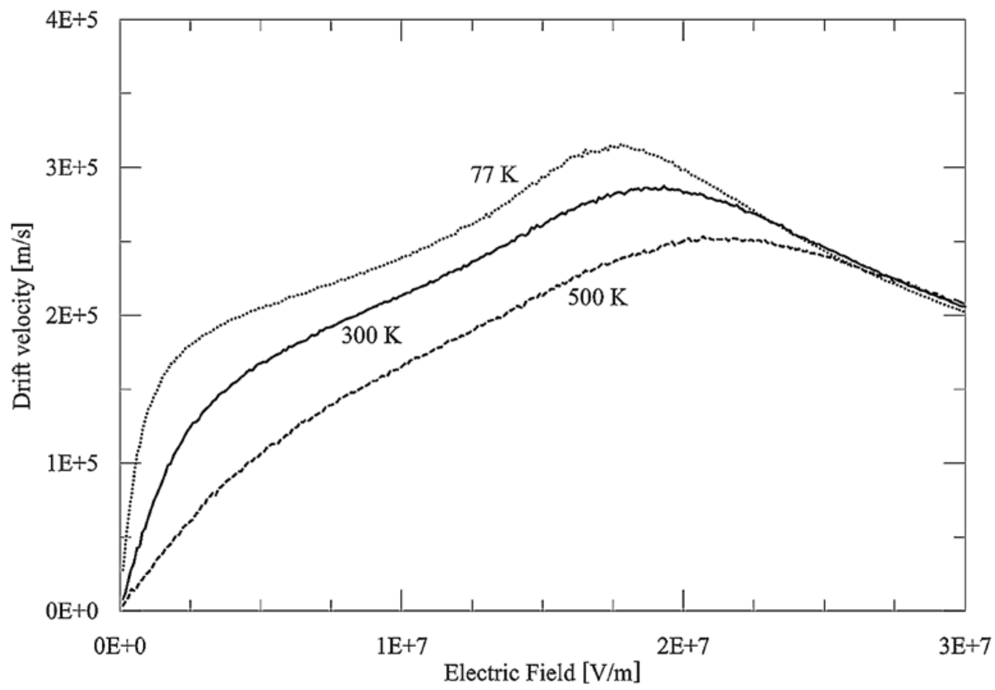


Fig. 1. – Temperature dependence of velocity-field characteristics of GaN.

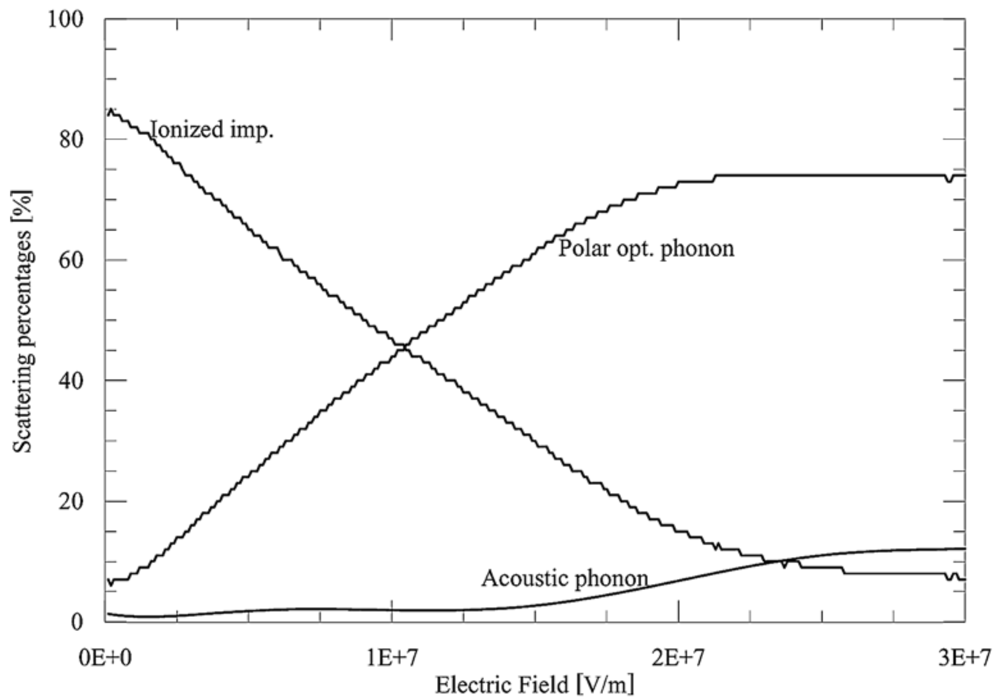


Fig. 2. – Scattering percentage of each mechanism in total scattering events in the simulation time of 2 ns as a function of the electric field for 300 K.