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Archives of Applied Science Research, 2010, 2 (1) 329-335
(http://scholarsresearchlibrary.com/archive.html)

ISSN 0975-508X
CODEN (USA) AASRC9

Influence of Temperature in High Field Electron Transport Properties in Bulk Wurtzite GaN

[1]H. Arabshahi and [2]M. Asmari

[1]Department of Physics, Ferdowsi University of Mashhad, Mashhad, Iran
[2]Climatology of Atmospheric Disasters Group, Climatological Research Institute, P.O. Box 91735–676, Mashad, Iran

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Abstract

An ensemble Monte Carlo simulation has been used to model bulk electron transport at room and higher temperatures as a function of high electric fields. Electronic states within the conduction band valleys at the Γ_1, U, M, Γ_3 and K are represented by non-parabolic ellipsoidal valleys centred on important symmetry points of the Brillouin zone. The simulation shows that intervalley electron transfer plays a dominant role in GaN in high electric fields leading to a strongly inverted electron distribution and to a large negative differential conductance. Our simulation results have also shown that the electron velocity in GaN is less sensitive to temperature than in other III-V semiconductors like GaAs. So GaN devices are expected be more tolerant to self-heating and high ambient temperature device modeling. Our steady state velocity-field characteristics are in fair agreement with other recent calculations.

Keywords: Ensemble Monte Carlo, brillouin zone, self-heating.

Introduction

Wide band gap GaN and related compounds with aluminium and indium currently have great potential for applications in high-power and optoelectronic devices. Blue light emitting GaN diode and heterojunction field effect transistors (HFETs) which can sustain high current densities at elevated temperatures have already been fabricated [1-2]. The Monte Carlo technique has proved valuable for studying non-equilibrium carrier transport in a range of semiconductor materials and devices [3-4], and electron transport in bulk GaN was modelled as long ago as 1975 [5]. However, carrier transport modelling of group III-nitrides has only recently begun to receive sustained attention [6-8], now that the growth of compounds and alloys is able to produce

viable material for the electronics industry. As the start of a programme of work modelling high field transport and breakdown in group III-nitrides, this paper presents the results of Monte Carlo simulations of electron transport in bulk GaN at different temperatures.

Most of the simulations have been carried out using a non-parabolic ellipsoidal valley model to describe transport in the conduction band. However, the simpler and less computationally intensive spherical parabolic band scheme has also been applied, to test the validity of this approximation. For the wurtzite GaN crystal structure, features associated with high field transport, in particular intervalley scattering and consequent electron velocity characteristics, are compared with that calculated for GaAs. This article is organised as follows.

Details of the conduction band parameters and the Monte Carlo simulation are presented in section 2, and the results of steady state and transient transport simulations are discussed in section 3.

Simulation Model

In this work, the two lowest energy conduction bands of the empirical pseudopotential band structure for wurtzite phase GaN is chosen as a basis of an analytical multivalley conduction band model. The pseudopotential band structure shows the conduction band minimum to be located at the Γ point (Γ_1), and lowest energy conduction band satellite valleys to occur at the U point (located about two thirds of the way between the L and M symmetry points) [9-10]. Higher conduction band valleys are located at the Γ point (Γ_3), at the M point, and at the K point. In our Monte Carlo simulation, the two different Γ_1 valleys, the six equivalent U valleys, the three equivalent M valleys, and the two equivalent K valleys, are represented by ellipsoidal, nonparabolic dispersion relationships of the following form [3-4]

$$E(k)[1+\alpha_i E(k)] = \frac{\hbar^2}{2}\left[\frac{k_x^2 + k_y^2}{m_\perp^*} + \frac{k_z^2}{m_\parallel^*}\right] \qquad (1)$$

where $m_\perp^*$ and $m_\parallel^*$ are the transverse and longitudinal effective masses at the band edge and α_i is the non-parabolicity coefficient of the i-th valley. The material parameters necessary for calculating the scattering probabilities used in the present Monte Carlo simulation are listed in table 1 [6-10]. Scattering mechanisms included in the simulation are acoustic deformation potential scattering (treated either as an elastic process or as an inelastic process) and pizoelectric scattering (which is found to be negligible in the temperature range discussed here). Furthermore, longitudinal optical phonon scattering, nonequivalent and, where applicable, equivalent intervalley scattering events are taken into account among all valley types with the transfers assumed to be governed by the same deformation potential fields and the same phonon frequencies. Degeneracy effects are expected to be negligible over almost all of the temperature and electron concentration ranges of interest here and, hence, are not considered in the calculation.

In our model at the start of each simulation, ten thousand electron particles are distributed in momentum space according to a Maxwell-Boltzmann distribution function. These particles are

propagated classically between collisions according to thier velocity, effective mass and the prevailing field. The selection of the propagation time, scattering mechanism and other related quantities is achieved by generating random numbers and using this numbers to select, for example, a scattering mechanism. In the case of the ellipsoidal, non-parabolic conduction valley model, the usual Herring-Vogt transformation matrices are used to map carrier momenta into spherical valleys when particles are drifted or scattered. Steady-state results of high field transport studies have been obtained for lattice temperatures up to 600 K, in order to gain some insight into the hot carrier transport and the energy distribution function that would be generated in the gate-drain region of a power field effect transistor.

Table 1. Material parameters used in the transport simulations

Parameter	Wurtzite GaN
Band-gap (eV)	3.5
Electron effective mass (m^*)	0.2
$m_{\parallel}^*$ (Γ-A)	0.18
$m_{\perp}^*$ (Γ - M)	0.189
Nonparabolicity (eV^{-1})	9.5
Static relative permitivity ε_0	5.35
Optical relative permitivity ε_∞	6150
Density (kgm^{-3})	4330
Sound velocity (ms^{-1})	8.3
Deformation potential (eV)	0.375
Piezoelectric constant (Cm^{-2})	0.0995
Optical phonon energy (eV)	

Simulation Results

Electron drift velocity as a function of electric field is important in determining the performance of high-speed and microwave semiconductor devices. Here we show the results of temperature dependence of the steady-state velocity-field characteristics and valley occupancy in the wurtzite phases of bulk GaN. Figure 1 shows the simulated velocity-field characteristics of wurtzite GaN at 300 K, with a background doping concentration of 10^{22} m^{-3}, and with the electric field applied along the hexagonal c-axis. In this figure, the solid curve represent simulation results obtained using non-parabolic valleys and the dashed curve are results obtained using parabolic bands.

The drift velocities obtained using both models agree within %5 but, by neglecting the non-parabolicity α, the average kinetic energy tends to be overestimated.

The simulations suggest that the peak drift velocity for wurtzite is ~2.3×10^5 ms^{-1}. At higher electric fields, intervalley optical phonon emission dominates, causing the drift velocity to saturate at around 2×10^5 ms^{-1}. The calculated high field electron drift velocity apparent from figure 1 is fractionally lower than those that have been calculated by Gelmont et al.[11], (e.g

2.3×10^5 ms^{-1} at an electric field ~1.4×10^7 Vm^{-1}) who assumed an effective mass in the upper valleys equal to the free electron mass. The threshold field for the onset of significant scattering into satellite conduction band valleys is a function of the intervalley separation and the density of electronic states in the satellite valleys.

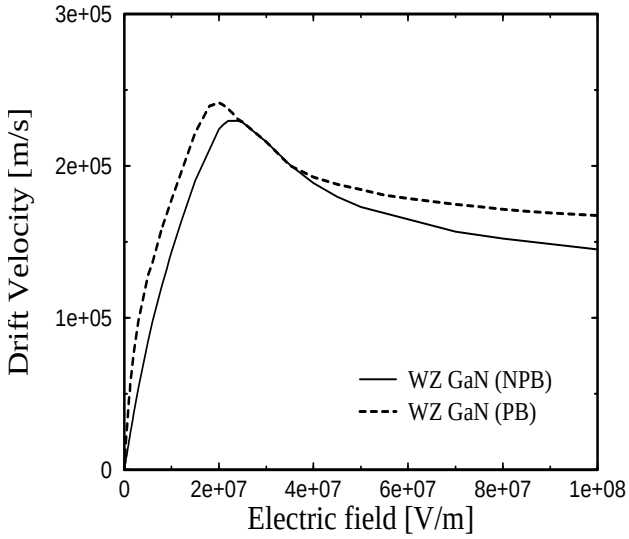

Figure 1: Calculated steady-state electron drift velocity in bulk wurtzite GaN using the parabolic (PB) and non-parabolic (NPB) band models

The importance of electron intervalley transfer at high electric fields can be clearly seen in figure 2. In this figure the fractional valley occupancies for wurtzite phase of GaN is plotted. It is obvious that the inclusion of satellite valleys in the simulations is important. Significant electron transfer to the upper valleys only begins to occur when the field strength is very close to the threshold value. At the threshold field the electron valley occupancies for Γ_1, U, K, M and Γ_3 are about %94, %5, %0.5, %0.3 and %0.2, respectively.

Figure 3 shows the calculated electron drift velocity as a function of electric field strength for temperatures of 300, 450 and 600 K. The decrease in drift mobility with temperature at low fields is due to increased intravalley polar optical phonon scattering whereas the decrease in velocity at higher fields is due to increased intra and intervalley scattering.

It can be seen from the figure that the peak velocity also decreases and moves to higher electric field as the temperature is increased.

This is due to the general increase of total scattering rate with temperature, which suppresses the electron energy and reduces the population of the satellite valleys.

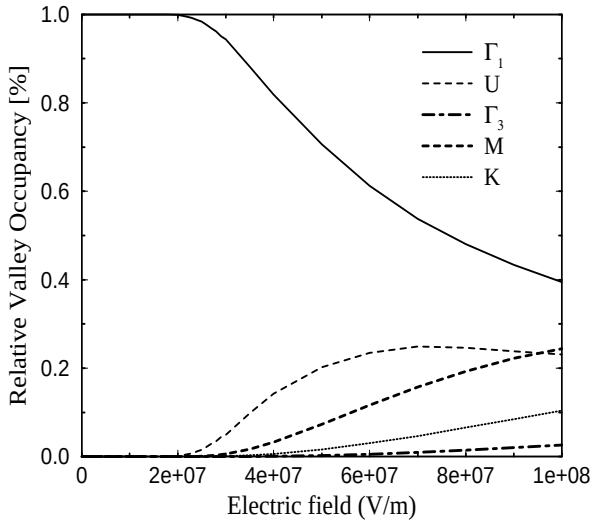

Figure 2. Fractional occupation of the central and satellite valleys of wurtzite GaN as a function of applied electric field using the non-parabolic band model at room temperature

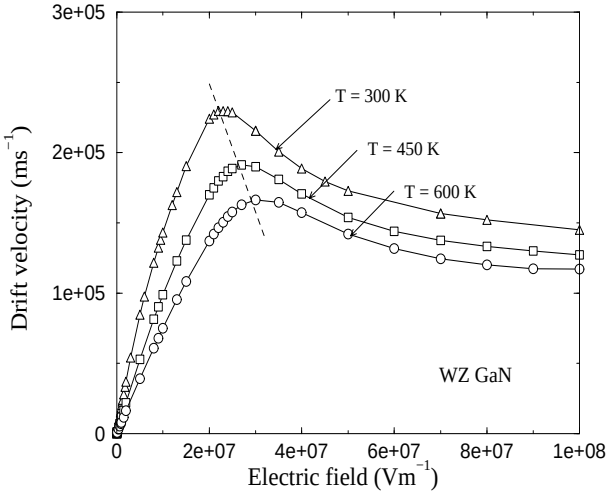

Figure 3. Calculated electron steady-state drift velocity in bulk wurtzite GaN as a function of applied electric field at various lattice temperatures and assuming a donor concentration of 10^{22} m^{-3}. The peak drift velocity decreases by about %20 while the threshold field increases by same percent as the lattice temperature increases from 300 to 600 K

This latter effect is apparent from the fact that the electron population in the Γ_1-valley increases with temperature as shown in figure 4. Figure 5 shows how the velocity-field relation changes with temperature for electrons in the most populated Γ_1 and U valleys. There are significant statistical fluctuations in the results for the drift velocity of electrons in the U valleys for fields around 2×10^7 Vm^{-1}, which are caused by the relatively small number of electron particles occupying the valleys just above the threshold for intervalley transfer. Nevertheless it can be seen that the average drift velocity decreases as the temperature increases for both valleys. Comparison of the temperature dependence of the transport properties in wurtzite GaN (figure 3) and GaAs (figure 6) shows that the change in peak velocity of GaN from 300 K to 600 K is a

reduction of about %35 whereas for GaAs it is about %78. Therefore, the electron velocity in GaN is less sensitive to temperature than in GaAs, and GaN devices are expected be more tolerant to self-heating and high ambient temperature.

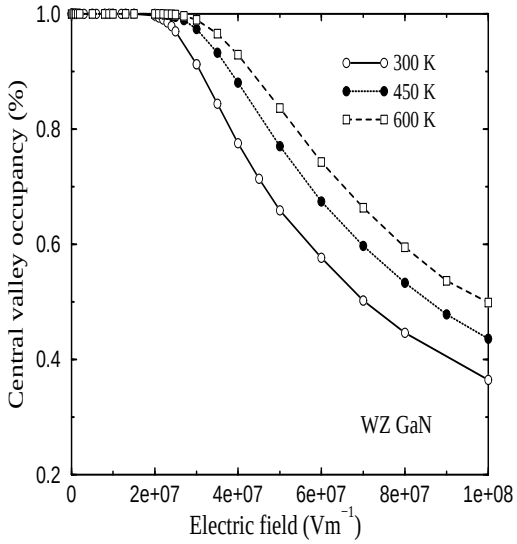

Figure 4. Fraction of electrons in the Γ_1 valley of wurtzite GaN as a function of applied electric field versus temperature

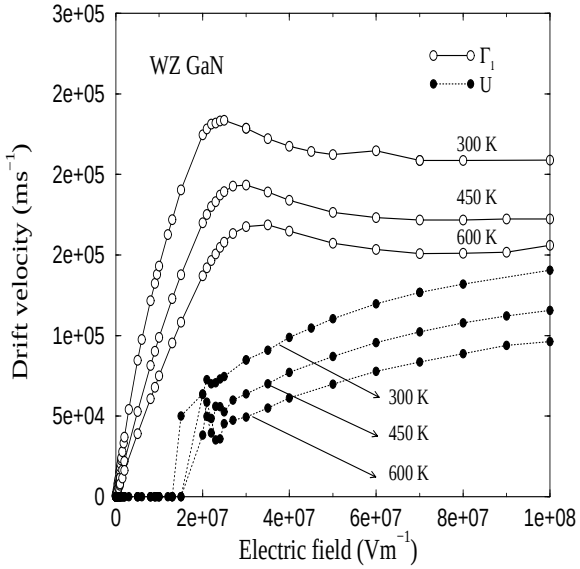

Figure 5. Temperature dependence of the drift velocity in the Γ_1 and U valleys in wurtzite GaN as functions of electric field

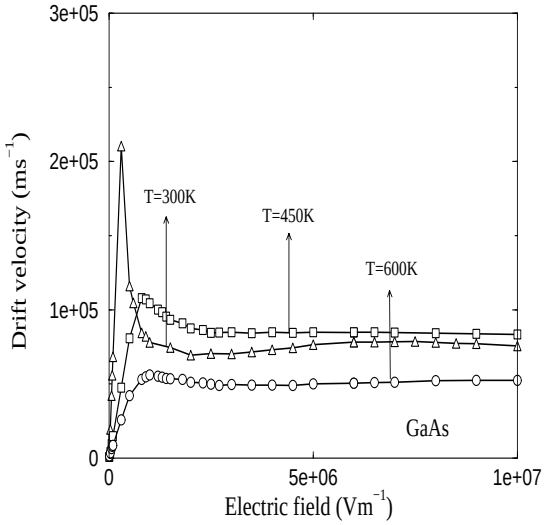

Figure 6. Calculated electron steady-state drift velocity in bulk GaAs as a function of applied electric field at various lattice temperatures and donor concentration of 10^{22} m^{-3}

Conclusion

Electron transport at different temperatures in bulk wurtzite GaN has been simulated using an ensemble Monte Carlo simulation. Using valley models to describe the electronic bandstructure, calculated velocity-field characteristics show that the intervalley transitions in high electric fields play an important role in GaN, in spite of a large separation between the central and upper valleys. The intervalley transitions lead to a large negative differential conductance. Saturation drift velocities of about 2×10^5 ms^{-1} match recent measurements on low-doped bulk samples. We have also demonstrated that low temperature sensitivity of the electron transport properties of wurtzite GaN is attractive for high-temperature and high-power electronic applications.

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