LOW-FIELD ELECTRON TRANSPORT PROPERTIES IN ZINCBLENDÉ AND WURTZITE GaN STRUCTURES USING AN ITERATION MODEL FOR SOLVING BOLTZMANN EQUATION

H. ARABSHAHI

Department of Physics, Tarbiat Moallem University of Sabzevar, P.O. Box 397, Sabzevar, Iran,
Department of Physics, Ferdowsi University of Mashhad, Mashhad, Iran
Email: hadi.arabshahi@sttu.ac.ir

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An iteration calculation has been carried out to study electron transport properties in zincblende and wurtzite GaN materials. The two-mode nature of the polar optic phonons is considered jointly with deformation potential acoustic, piezoelectric, ionized impurity scattering. Band nonparabolicity, admixture of p functions, arbitrary degeneracy of the electron distribution, and the screening effects of free carriers on the scattering probabilities are incorporated. Electron drift mobility in both zincblende and wurtzite GaN crystal structures are calculated for different temperature and doping dependencies. It is found that the electron mobility decreases monotonically as the temperature increases from 100 K to 600 K. The low temperature value of electron mobility increases significantly with increasing doping concentration. The agreement of iterative results with the available experimental data is found to be satisfactory.

Keywords: Iterative, deformation potential, piezoelectric, nonparabolicity, mobility.

1. INTRODUCTION

Gallium nitride has long been considered promising material for electronic and optoelectronic device applications [1–4]. The wide and direct energy gap, large breakdown field, high thermal conductivity, and favorable electron-transport characteristics, make the GaN ideally suited for high-power and high-speed applications. While initial efforts to study this material was hindered by growth difficulties, recent improvements in the material quality have made possible the realization of a number of GaN-based devices. In particular, lasers [5], transistors and photodetectors [6] have been fabricated with these materials. These developments have fueled considerable interest in the GaN material. In order to analyze and improve the design of GaN-based devices, an understanding of the electron transport that occurs within these materials is necessary. While electron transport in bulk GaN has been extensively examined [7–9], the
sensitivity of these results to variations in the material parameters has yet to be considered.

This paper presents the iterative calculation results of electron transport in bulk GaN materials. Most of the calculations have been carried out using a nonparabolic 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. The iterative calculations take into account the electron-lattice interaction through polar optical phonon scattering, deformation potential acoustic phonon scattering (treated as an elastic process), piezoelectric and electron-plasmon scattering. Impurity scattering due to ionized and neutral donors is also included, with the latter found to be important at low temperature due to the relatively large donor binding energy which implies considerable carrier freeze-out already at low temperature. This paper is organised as follows.

Details of the iterative model and the electron mobility calculations are presented in section 2 and the results of iterative calculations carried out on GaN structures are interpreted in section 3.

2. MODEL DETAILS

In principle the iterative and Monte Carlo techniques give exact numerical predictions of electron transport phenomena in bulk semiconductors [10–11]. Both of them can include the details of the microscopic electronic processes and can be extended to time-dependent phenomena. In low electric fields the effects of scattering, which depend on the details of the distribution function, can be dealt with more conveniently by the iterative technique because it processes the whole distribution function at each step of the procedure. In contrast the Monte Carlo method is highly susceptible to statistic fluctuations in the ensemble when the departure from equilibrium is small because of the weakness of the electric field effects [12–14]. For these reasons, we used the iterative method to determine the low field electron mobility in bulk GaN.

Rode’s iterative technique provides a compact method of solution of the Boltzmann equation in the low field regime [15–17]. The Boltzmann transport equation for the distribution function $f(r, k, t)$ is

$$\frac{\partial f}{\partial t} + v \cdot \nabla_r f + \frac{qF}{h} \cdot \nabla_k f = \left( \frac{\partial f}{\partial t} \right)_{coll}$$  \hspace{1cm} (1)

where $\left( \frac{\partial f}{\partial t} \right)_{coll}$ represents the change of distribution function due to the electron scattering. In the steady-state and under application of a uniform electric field the Boltzmann equation can be written as
Consider electrons in an isotropic, non-parabolic conduction band whose equilibrium Fermi distribution function is \( f_0(k) \) in the absence of electric field. Note the equilibrium distribution \( f_0(k) \) is isotropic in \( k \) space but is perturbed when an electric field is applied. If the electric field is small, we can treat the change from the equilibrium distribution function as a perturbation which is first order in the electric field. The distribution in the presence of a sufficiently small field can be written quite generally as

\[
f(k) = f_0(k) + f_1(k) \cos \theta \tag{3}\]

where \( \theta \) is the angle between \( k \) and \( F \) and \( f_1(k) \) is an isotropic function of \( k \), which is proportional to the magnitude of the electric field. \( f(k) \) satisfies the Boltzmann equation 2 and it follows that

\[
\frac{eF}{\hbar} \equiv \frac{\partial f_0}{\partial k} = \sum_i \left[ \int \cos \theta' f_i'(s_i'(1-f_0') + s_i f_0') d^3k' - f_i \cos \theta \int [s_i(1-f_0') + s_i' f_0'] d^3k' \right] \tag{4}\]

where the sum is over scattering processes \( i \). For a more compact notation we have written \( f(k') = f' \), \( s_i(k, k') = s_i \) and \( s_i(k', k) = s_i' \). \( s_i(k, k') = s_i \) is the probability for scattering out of state \( k \) into the differential element \( d^3k' \) at \( k' \). For the isotropic conduction band \( s_i(k, k') \) depends on only \( k \) and the cosine of the angle \( \phi \) between them, and the relation

\[
\int \cos \theta' A(\cos \phi) d^3k' = \cos \theta \int \cos \phi A(\cos \phi) d^3k' \tag{5}\]

may be used to manipulate equation 4. Here \( A(\cos \phi) \) is an arbitrary function of \( \cos \phi \) but does not otherwise depend on \( \theta \) and \( \theta' \). From equation 4 and 5 we obtain

\[
\frac{eF}{\hbar} \equiv \frac{\partial f_0}{\partial k} = \sum_i \left[ \int \cos \phi f_i'(s_i'(1-f_0') + s_i f_0') d^3k' - f_i \int [s_i(1-f_0') + s_i' f_0'] d^3k' \right] \tag{6}\]

In general there will be both elastic and inelastic scattering processes. For example impurity scattering is elastic and acoustic and piezoelectric scattering are elastic to a good approximation at room temperature. However, polar and non-polar optical phonon scattering are inelastic. Labelling the elastic and
inelastic scattering rates with subscripts $el$ and $inel$ respectively and recognising that, for any process $i$, $s_{el}(k', k) = s_{eli}(k, k')$ equation 6 can be written as

$$f_j(k) = \frac{(-eF / h)(\partial f_0 / \partial k) + \sum_j \int \cos \phi f_0 \left[s_{inel}^0(1 - f_0) + s_{inel} f_0 \right] d^3k'}{\sum_j \int (1 - \cos \phi) s_{el} d^3k' + \sum_j \int [s_{inel}^0(1 - f_0) + s_{inel}^0 f_0] d^3k'}$$  (7)

Note the first term in the denominator is simply the momentum relaxation rate for elastic scattering. Equation 7 may be solved iteratively by the relation

$$f_{in}(k) = \frac{(-eF / h)(\partial f_0 / \partial k) + \sum_j \int \cos \phi f_0 \left[s_{inel}^0(1 - f_0) + s_{inel} f_0 \right] d^3k'}{\sum_j \int (1 - \cos \phi) s_{el} d^3k' + \sum_j \int [s_{inel}^0(1 - f_0) + s_{inel}^0 f_0] d^3k'}$$  (8)

where $f_{in}(k)$ is the perturbation to the distribution function after the $n$-th iteration. It is interesting to note that if the initial distribution is chosen to be the equilibrium distribution, for which $f(k)$ is equal to zero, we get the relaxation time approximation result after the first iteration. We have found that convergence can normally be achieved after only a few iterations for small electric fields. Once $f(k)$ has been evaluated to the required accuracy, it is possible to calculate quantities such as the drift mobility $\mu$, which is given by

$$\mu = \frac{\int \mathbf{v} \cdot \mathbf{F} f(k) d^3k}{\int f(k) d^3k}$$  (9)

In terms of spherical coordinates

$$\mu = \frac{\int_0^\infty v k^2 (f_1 / F) dk}{3 \int_0^\infty k^2 f_0 dk}$$  (10)

The Kane approximation relation [18] between electron group velocity and effective mass $m'$ in a nonparabolic band is

$$v(k) = \frac{\hbar k}{m' (1 + 2\alpha E)}$$  (11)

and substituting this result in equation 10 we find that

$$\mu = \frac{\hbar}{3m' F} \int_0^\infty \frac{k^3 / (1 + 2\alpha E) f_1 dk}{\int_0^\infty k^2 f_0 dk}$$  (12)
Here, we have calculated low field drift mobility in GaN structures using the iterative technique. The effects of piezoelectric, acoustic deformation, polar optical phonons and ionized impurity scattering have been included in the model. It is also assumed that the electrons remain in the $\Gamma$-valley of the Brillouin zone. The valley is isotropic in the case of zincblende GaN and approximated as such for the wurtzite crystal structure.

3. LOW-FIELD TRANSPORT RESULTS IN BULK GaN

We have performed a series of low-field electron mobility calculations for both GaN structures. Low-field mobilities have been derived using iteration methode. Important parameters used throughout the calculations are listed in Table 1, which are taken from Ref. [13, 14]. Fig. 1 shows the calculated electron drift mobilities versus temperature and donor concentration for zincblende and wurtzite GaN. The electron drift mobilities at room temperature that we find are 1300 and 900 cm$^2$V$^{-1}$s$^{-1}$ for zincblende and wurtzite structures, respectively, for an electric field equal to $10^4$ Vm$^{-1}$ and with a donor concentration of $10^{22}$ m$^{-3}$. The material parameters used to calculate the electron drift mobilities are tabulated in Table 1. For the wurtzite crystal structure it is assumed that the conduction band is isotropic with an effective mass $0.2m_0$. This is a reasonable approximation since $m_i^* \approx m_e^*$ and $m_i^*$ differ by only 10%.

Table 1

<table>
<thead>
<tr>
<th>Important parameters used in our calculations for zincblende and wurtzite GaN materials</th>
<th>Zb-GaN</th>
<th>Wz-GaN</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density $\rho$ [kgm$^{-3}$]</td>
<td>6100</td>
<td>6150</td>
</tr>
<tr>
<td>Longitudinal sound velocity $v_L$ (ms$^{-1}$)</td>
<td>4570</td>
<td>4330</td>
</tr>
<tr>
<td>Low-frequency dielectric constant $\varepsilon_\infty$</td>
<td>9.5</td>
<td>9.5</td>
</tr>
<tr>
<td>High-frequency dielectric constant $\varepsilon_\infty$'</td>
<td>5.35</td>
<td>5.35</td>
</tr>
<tr>
<td>Acoustic deformation potential $D$ [eV]</td>
<td>8.3</td>
<td>8.3</td>
</tr>
<tr>
<td>Polar optical phonon energy $\hbar \omega_{op}$ [meV]</td>
<td>99</td>
<td>99</td>
</tr>
<tr>
<td>Bandgap $E_g$ [meV]</td>
<td>3.2</td>
<td>3.5</td>
</tr>
<tr>
<td>Nonparabolicity $\alpha$ [eV$^{-1}$]</td>
<td>0.213</td>
<td>0.189</td>
</tr>
<tr>
<td>Electron effective mass:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$m_i^*$ ($\Gamma$-A direction)</td>
<td>0.15</td>
<td>0.18</td>
</tr>
<tr>
<td>$m_i^*$ ($\Gamma$-M direction)</td>
<td>0.15</td>
<td>0.2</td>
</tr>
</tbody>
</table>

The results plotted in Fig. 1a indicate that the electron drift mobility of wurtzite GaN is lower than that for the zincblende structure at all temperatures. This is largely due to the higher $\Gamma$ valley effective mass in the wurtzite phase.
Fig. 1 – (a) Electron drift mobility of GaN in zincblende and wurtzite structures versus temperature. Donor concentration is approximately $10^{22}$ m$^{-3}$, (b) Electron drift mobility of GaN in zincblende and wurtzite structures versus donor concentration at room temperature. Fig. 1b shows the calculated variation of the electron mobility as a function of the donor concentration for both GaN crystal structures at room temperature. The mobility does not vary monotonically between donor concentrations of $10^{21}$ and $10^{25}$ m$^{-3}$ due to the dependence of electron scattering on donor concentration, but shows a maximum near $10^{21}$ m$^{-3}$ for zincblende and wurtzite. In order to understand the scattering mechanisms which limit the mobility of GaN under various conditions, we have performed calculations of the electron drift mobility when particular scattering processes are ignored. The solid curve in Fig. 2 shows the calculated mobility for wurtzite GaN including all scattering mechanisms whereas the dashed, dotted, and open circle curves show the calculated mobility without ionized impurity, piezoelectric and polar optical scattering, respectively. It can be seen that below 300 K the ionized impurity scattering is dominant while at the higher temperatures electron scattering is predominantly by optical modes. Thus the marked reduction in mobility at low temperatures seen in Fig. 2 can be ascribed to impurity scattering and that at high temperatures to polar optical phonon scattering. In Fig. 2 the mobility in the absence of band non-parabolicity is plotted as a dash-dot curve. Nonparabolicity leads to approximately a 10% reduction relative to the mobility for parabolic band at room temperature. This is because nonparabolicity increases the electron effective mass and also the scattering rates through the density of states. The temperature variation of the electron drift mobility in zincblende and wurtzite
GaN for different donor concentrations is shown in Fig. 3. It is evident from this figure that the curves approach each other at very high temperatures, where the mobility is limited by longitudinal optical phonon scattering, whereas the mobility varies inversely with donor concentration at low temperatures as we would expect from the foregoing discussion.

Finally, we compare the drift mobility characteristics of GaAs, as shown in Fig. 4 with those of GaN. The drift mobility characteristics of the two materials show similar trends, reflecting the fact that both materials are direct-gap
compound semiconductors. However, the mobility in GaAs is \(7200 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}\) at 300 K, some 5 times greater than for zincblende GaN. This is a consequence of the smaller \(\Gamma\)-valley effective mass, 0.068 \(m_0\) \textit{(versus} 0.15 \(m_0\) in zincblende GaN) and small polar optical phonon energy 0.036 eV in GaAs \textit{(versus} 0.099 eV in zincblende GaN).

Fig. 4 – (a) Electron drift mobility of GaAs \textit{versus} temperature for different donor concentrations. The solid, long-dashed lines represent the results for \(10^{22}\), \(5 \times 10^{22}\) and \(10^{23}\) \(\text{m}^{-3}\), respectively, (b) Electron drift mobility of GaAs \textit{versus} donor concentration at different temperatures.

4. CONCLUSIONS

In conclusion, we have studied the electron transport characteristic associated with zincblende and wurtzite GaN. Temperature dependent and free electron concentration dependent of the electron mobility in both GaN structures have been compared. It has been found that the low-field electron mobility is significantly higher for the zincblende GaN structure than zincblende structure due to the lower \(\Gamma\) electron effective mass in this crystal structure. Several scattering mechanisms have been included in the calculation. Ionized impurities have been treated beyond the Born approximation using a phase shift analysis. Screening of ionized impurities has been treated more realistically using a multi-ion screening formalism, which is more relevant in the case of highly compensated III–V semiconductors like GaN.

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REFERENCES