Anisotropic longitudinal electron diffusion coefficient in wurtzite gallium nitride

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Abstract The longitudinal electron diffusion coefficient ($D_l$) of wurtzite (WZ) gallium nitride (GaN) is calculated by an ensemble Monte Carlo (EMC) method. By using the power spectral density associated with velocity fluctuation, the relationship between $D_l$ and electric field strength, frequency, doping concentration and temperature is presented. The anisotropic $D_l$ of GaN impacted by anisotropy of the electronic dispersion is also investigated. It has been found that the $D_l$ in $\Gamma$–$A$ direction (c-direction) is larger than that in $\Gamma$–$M$ direction (basal plane) in most cases. For lower electric field, the $D_l$ keeps constant at first, then decreases with increasing frequency. However, for higher electric field, the $D_l$ firstly approaches a peak value, then decreases with increasing frequency. When the frequency is zero, the $D_l$ decreases with increasing electric field, and then increases until a peak value. Finally, it decreases with increasing electric field again. When the temperature increases, the $D_l$ decreases in both directions for increasing scattering rate. A comparison between our calculated diffusion coefficient and the mobility under low electric field by Einstein equation is presented.

1 Introduction

As a wide-band gap semiconductor and a promising candidate in semiconductor device, GaN material has shown potential application in millimeter-wave, solar cells, and optoelectronic devices, which have been researched widely in the past few years [1–6]. To make a clear description and an understanding of the working theory of the devices, the transport property of GaN has been researched a lot, which includes the experiments and theory simulations, especially the velocity-field relation [7–9] or electron mobility calculation [10–12]. In addition to the drift velocity, the diffusion coefficient is also an important parameter in the fundamental theoretical model of the material, which has not been paid much attention. The widely used diffusion coefficient is deduced from the Einstein equation by mobility. However, the Einstein equation can only hold at low electric field when the Boltzmann distribution is satisfied [13, 14]. Moreover, much work assumes an isotropic electronic structure of GaN [8, 10, 11]. Some researches are based on anisotropy of electronic dispersion of GaN [7, 9], which mainly concerns about the velocity-field relation. And recent experiments have shown the anisotropic transport characteristics of GaN [15, 16]. The anisotropic electron diffusion coefficient is still an unsolved question. And these works based on anisotropy of electronic dispersion of GaN have clearly shown that the transport properties will change a lot for the anisotropic energy structure. This motivate our work consider the effect of anisotropy of electronic dispersion of GaN to the electron diffusion coefficient.

Some researches on GaAs, InP, and Si show that diffusion coefficient changes obviously with varying electric field strength, frequency, carrier concentration and temperature [17–20]. For the reasons above and the importance of diffusion coefficient in the simulation of solid-state devices, the electron diffusion coefficient in wurtzite GaN as the function of the electric field strength, frequency, carrier concentration and temperature is investigated by an EMC simulation. The anisotropy of diffusion coefficient caused by the anisotropy of the electronic dispersion is also presented. The widely used diffusion coefficient in device simulation is longitudi-
nal electron diffusion coefficient, and the transverse diffusion coefficient is not included.

By using the power spectral density associated with velocity fluctuations and the autocorrelation function, the paper investigates the relationship between the anisotropic longitudinal electron diffusion coefficient and the electric field strength, frequency, carrier concentration, and temperature. Details of the Monte Carlo procedure are presented in Sect. 2. The definition of diffusion coefficient by autocorrelation function is also given in this part. In Sect. 3 the simulation results are discussed. First, the steady state velocity-field relationship and the electrons occupied rate in three valleys are presented to make a clear description of the electrons transport property. Next, we discuss the feature of autocorrelation function in $\Gamma$–A direction. By using autocorrelation function, we obtain the electron diffusion coefficient in $\Gamma$–A and $\Gamma$–M directions as the function of frequency under different electric field. The anisotropy of diffusion coefficient as a function of electric field is also presented. By using different scattering mechanism, we explain the variation curve of the $D_l$. Moreover, the $D_l$ as a function of electric field is investigated, and the zero-field mobility can be deduced by the Einstein equation. Finally, the influence of temperature on $D_l$ is presented in two different directions. Conclusions are presented in Sect. 3.

2 Simulations model

The $D_l$ used in simulation software is deduced from the well-known Einstein equation, which can only hold in the line-response regime of the velocity-field relation curve, as shown in Eq. (1).

$$D = \frac{1}{q}\mu K_b T$$

where $q$ is electronic charge, $K_b$ is the Boltzmann constant, and $T$ is the temperature. However, the result obtained by this method is impacted by two factors. On one hand, MC calculation is become less accurate for the drift velocity obtained from the average velocity of the “sample” electron at the lower field, which is only a small fraction of the thermal velocity when the electric field tends to be zero. On the other hand, at higher electric field, the Einstein equation will no longer hold for the distribution function deviated from the Boltzmann distribution [13, 14]. The diffusion coefficient must be calculated by other means. Some researches have shown that the diffusion coefficient reflects the velocity fluctuations suffered by carriers. It can be calculated by the power spectral density associated with velocity fluctuations, as shown in Eq. (2) [21, 22].

$$D(w) = \int_0^\infty C(t) \cos(\omega t) \, dt$$

where $C(t)$ is autocorrelation function. $C(t)$ is defined by Eq. (3).

$$C(t) = \left[ \langle v(t') - \langle v \rangle \rangle \langle v(t' + t) - \langle v \rangle \right]$$

where $v(t')$ is the drift velocity at time $t'$, $\langle v \rangle$ is the average drift velocity. The bracket indicates time average, which can be calculated by ensemble average.

In MC method, the motion of electrons is accelerated by the electric field. The electrons are scattered by the random scattering mechanism. The MC technique can obtain all the information on the stochastic motions of electrons in the semiconductor. Therefore, the diffusion coefficient can be obtained by MC method. A nonparabolic three-valley model with the conduction band minima located at $\Gamma^1$, $U$, and $\Gamma^3$ points in the Brillouin zone is adopted in the EMC calculation. The scattering mechanisms include the deformation potential, polar optical phonon interactions, and intervalley deformation potential scattering. The scattering with ionized impurities uses the Brooks–Herring method [23]. To simulate the effect of the anisotropy of band structure, Herring–Vogt transformation [24] is adopted in EMC simulation. The material parameters of wurtzite GaN are collected by the published references [8, 11, 25, 26], as shown in Table 1. The nonparabolicity is included in the electronic dispersion relationship as follows:

$$\frac{\hbar^2 k^2}{2m} = \varepsilon(1 + \alpha \varepsilon)$$

where $\alpha$ is the nonparabolicity, $m$ is the effective mass, $\varepsilon$ represents the energy.

3 Simulation results of Monte Carlo

In this section, we present the simulation results of Monte Carlo simulations of electron transport in wurtzite gallium nitride. Figure 1 shows the steady-state electron drift velocity in GaN as a function of the applied electric field in $\Gamma$–M and $\Gamma$–A directions. The electrons occupancy of the central ($\Gamma^1$) and satellite valleys ($U$, $\Gamma^3$) are presented. It can be found that the steady-state electron drift velocity in $\Gamma$–M direction is different from that in $\Gamma$–A direction. The peak velocity is attained at $E = 200$ kV/cm and 240 kV/cm for $\Gamma$–A and $\Gamma$–M direction, respectively. When the electric field is smaller, the velocity is almost the same for two different directions. However, the slope shows much difference. The slope represents the mobility, which can be obtained by calculating diffusion coefficient. The difference comes from the different effective mass in two directions, as shown in Table 1. The difference in two directions becomes smaller with increasing electric field. The coupled effect of effective mass in the satellite valleys and strong intervalley scattering reduces the influence of the effective mass. For the different transport properties in two directions, it is essential to
**Table 1** Parameters used in EMC simulation

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass density (\rho) (g/cm(^3))</td>
<td>6.087</td>
</tr>
<tr>
<td>Sound velocity (10(^5) cm/s)</td>
<td>7.619</td>
</tr>
<tr>
<td>Low frequency dielectric constant</td>
<td>9.7</td>
</tr>
<tr>
<td>High frequency dielectric constant</td>
<td>5.28</td>
</tr>
<tr>
<td>Acoustic deformation potential (eV)</td>
<td>8.3</td>
</tr>
<tr>
<td>Polar optical phonon energy (eV)</td>
<td>0.092</td>
</tr>
<tr>
<td>Intervaly deformation potential, (Dij) (eV/cm)</td>
<td>65.8361</td>
</tr>
<tr>
<td>Piezoelectric constant, (e_{14}) (10(^{-5}) C/cm(^2))</td>
<td>3.75</td>
</tr>
<tr>
<td>Band gap (eV)</td>
<td>3.4</td>
</tr>
<tr>
<td>Effective mass (m_{\parallel}) ((\Gamma^1, U,\text{ and } \Gamma^3\text{ valley}))</td>
<td>0.1846, 0.3858, 0.2856</td>
</tr>
<tr>
<td>Effective mass (m_{\perp}) ((\Gamma^1, U,\text{ and } \Gamma^3\text{ valley}))</td>
<td>0.2283, 0.3858, 0.2856</td>
</tr>
<tr>
<td>Energy separation of WZ GaN (eV)</td>
<td>0.0, 2.2717, 2.4</td>
</tr>
<tr>
<td>Nonparabolicity of WZ GaN (eV(^{-1})) ((\Gamma^1, U,\text{ and } \Gamma^3\text{ valley}))</td>
<td>0.37, 0.385, 0.22</td>
</tr>
</tbody>
</table>

**Fig. 1** Room-temperature steady-state velocity-field characteristics and occupancy of the central (\(\Gamma^1\)) and satellite valleys (\(U, \Gamma^3\)) of wurtzite GaN when the electric field is in \(\Gamma^\text{–}M\) and \(\Gamma^\text{–}A\) directions. The peak velocity is attained at \(E = 200 \text{ kV/cm and } 240 \text{ kV/cm}\) for \(\Gamma^\text{–}A\) and \(\Gamma^\text{–}M\) directions, respectively. The doping level is \(1 \times 10^{17} \text{ cm}^{-3}\) and the temperature is 300 K

**Fig. 2** Longitudinal velocity autocorrelation function for electrons in wurtzite GaN in \(\Gamma^\text{–}A\) direction for different electric field (10 kV/cm, 40 kV/cm, 80 kV/cm, 150 kV/cm, 200 kV/cm, 500 kV/cm). The doping level is \(1 \times 10^{17} \text{ cm}^{-3}\) and the temperature is 300 K

consider the influence of anisotropic energy band of GaN in calculating the electron diffusion coefficient.

Figure 2 shows longitudinal velocity autocorrelation function \((Cp(t))\) for electrons in wurtzite GaN in \(\Gamma^\text{–}A\) for electric field 10 kV/cm, 40 kV/cm, 80 kV/cm, 150 kV/cm, 200 kV/cm, 500 kV/cm, respectively. The \(Cp(t)\) in \(\Gamma^\text{–}M\) has the same tendency, which is not shown here. The results are calculated by Eq. (4). The \(Cp(t)\) decreases sharply at the initial time. It denotes that velocity loses the correlation quickly. When the electric field is bigger, the \(Cp(t)\) becomes negative and finally approaches zero. The existence of negative value of \(Cp(t)\) was explained in [27] to be due to intercollision periods during which the fluctuation changes from negative to positive values due to its nearly linear increase with time. The correlation time (while \(Cp(t)\) becomes zero) will become smaller as the increasing electric field for the increasing scattering rate as the increasing electric field. It must be noted that the \(Cp(t)\) is sensitive to the velocity fluctuations. So, 30,000 electrons and a time step of \(1 \times 10^{-14} \text{ s}\) are adopted in the EMC simulation.

Figure 3 shows longitudinal diffusion coefficient \(D_l(\omega)\) versus frequency for wurtzite GaN in \(\Gamma^\text{–}A\) and \(\Gamma^\text{–}M\) directions at different electric field. The electric field is 1 kV/cm, 5 kV/cm, 10 kV/cm, 40 kV/cm, 100 kV/cm, 150 kV/cm, 200 kV/cm, 300 kV/cm, 400 kV/cm, and 500 kV/cm, respectively. \(D_l(\omega)\) is calculated from the autocorrelation function by Eq. (2), and the doping concentration is \(1 \times 10^{17} \text{ cm}^{-3}\). \(D_l(\omega)\) keeps constant at lower frequency. However, at higher frequency, \(D_l(\omega)\) shows different property for different electric field. When the electric field is small, \(D_l(\omega)\) decreases as the increasing frequency, while the electric field is high \(D_l(\omega)\) firstly increases to a peak and then decreases exponentially. The difference may come from the contribution of intervalley scattering. For higher electric
Fig. 3 Longitudinal diffusion coefficient $D_l(\omega)$ versus frequency for GaN at different electric field. (a) $\Gamma$–$A$ direction, (b) $\Gamma$–$M$ direction. The doping concentration is $1.0 \times 10^{17}$ cm$^{-3}$ and the temperature is 300 K.

Fig. 4 (a) Diffusion coefficient as the function of electric field and average energy of the lowest valley in $\Gamma$–$A$ and $\Gamma$–$M$ directions at 300 K, respectively. The doping concentration is $1.0 \times 10^{17}$ cm$^{-3}$. The frequency is zero. (b) Scattering rate in the lowest valley: 1, coulomb scattering; 2, piezoelectric; 3, phonon deformation potential; 4, polar optical phonon (absorb); 5, polar optical phonon (emission).

Field, the value of $D_l(\omega)$ is smaller at low frequency and the maximum diffusion coefficient occurs at higher frequency. It can also find that the $D_l(\omega)$ in $\Gamma$–$A$ direction is bigger than that in the $\Gamma$–$M$ direction, which is caused by the smaller effective mass in $\Gamma$–$A$ direction.

Figure 4(a) shows the $D_l$ in $\Gamma$–$M$ and $\Gamma$–$A$ directions, respectively. When the electric field is lower, the $D_l$ becomes smaller, approaches a minimum value, and then increases to a maximum value with increasing electric field. Finally, it decreases again with increasing electric field. Previous research on InP has observed the same tendency. However, the reason leading to the minimum $D_l$ has not been found [17]. There is no intervalley scattering at the minimum position, as shown in Fig. 1. So, the intervalley scattering begins at about 1.4 kV/cm and has no influence on the phenomenon. When the electric field is lower than 1.4 kV/cm, the mainly scattering mechanisms are ionized impurity, acoustic deformation potential, piezoelectric and polar optical phonon scattering, as shown in Fig. 4(b). The drift velocity of electrons increases when the electric field increases, as shown in Fig. 1. The velocity correlation decreases for higher velocity when the electrons are scattered. According to Eq. (2), the $D_l$ decreases with increasing electric field. However, when the electric field continues increasing, the average energy of electrons increases. And the polar optical phonon scattering will be the dominating scattering mechanism, which will become small anger scattering when the energy is large enough. When electrons are scattered by polar optical phonon, they keep most of their velocity correlation. The $D_l$ calculated by Eq. (2) will increase as the increasing electric field. Finally, it approaches a maximum value. When the electric field continue increasing, the intervalley scattering, which is isotropic scattering, will become the dominating scattering and the $D_l$ will decrease as the increasing electric field. What is more, the minimum of $D_l$ will come at a relative small electric field in $\Gamma$–$A$ direction for the smaller effective mass and their bigger average drift velocity as shown in Fig. 1. However, the peak of $D_l$ in $\Gamma$–$A$ direction will come earlier for the larger average energy, which comes from the smaller electron effective mass and the electrons can be more easily accelerated.

Table 2 shows the electron diffusion coefficient calculated by the traditional velocity-field curve shown in Fig. 1. The diffusion coefficient shows larger difference when the electric field increases. Even when the electric field is not large, the results calculated by the two different methods is

\[ \begin{align*}
D_l(\omega) & \approx \frac{1}{\lambda_1} \\
& \approx \frac{1}{\lambda_2} \\
& \approx \frac{1}{\lambda_3} \\
& \approx \lambda_4 \\
& \approx \lambda_5
\end{align*} \]
The electron diffusion coefficient calculated by Einstein equation and autocorrelation function (cm²/s)

<table>
<thead>
<tr>
<th></th>
<th>1 kV/cm</th>
<th>10 kV/cm</th>
<th>40 kV/cm</th>
<th>150 kV/cm</th>
<th>300 kV/cm</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Gamma$–A (Einstein equation)</td>
<td>25.610</td>
<td>19.944</td>
<td>10.805</td>
<td>4.681</td>
<td>2.243</td>
</tr>
<tr>
<td>$\Gamma$–A (Autocorrelation function)</td>
<td>27</td>
<td>20</td>
<td>7.483</td>
<td>10.0</td>
<td>5.101</td>
</tr>
<tr>
<td>$\Gamma$–M (Einstein equation)</td>
<td>20.717</td>
<td>17.205</td>
<td>9.296</td>
<td>4.002</td>
<td>2.151</td>
</tr>
<tr>
<td>$\Gamma$–M (Autocorrelation function)</td>
<td>23</td>
<td>17</td>
<td>6.957</td>
<td>7.715</td>
<td>4.218</td>
</tr>
</tbody>
</table>

The frequency is zero obviously different. The results show that the diffusion coefficient must be calculated by other means for higher electric field.

Figure 5(a) shows the $D_l$ as a function of doping density without electric field at 300 K in $\Gamma$–M and $\Gamma$–A directions, respectively. For lower doping concentration, the diffusion coefficient keeps constant for the piezoelectric and polar optical phonon scattering, which is not sensitive to doping concentration. When doping concentration decreases, the piezoelectric scattering rate increases slightly for the weakening shielding effect, and the diffusion coefficient decreases lightly, as shown in Fig. 5(a), which has been ignored in earlier transport property. The diffusion coefficient is influenced by the ionized impurity scattering for higher doping concentration. It decreases with increasing doping concentration. The $D_l$ in $\Gamma$–A direction is smaller than that in $\Gamma$–M direction, which is attributed to the larger effective mass in $\Gamma$–M direction.

We can get the zero-field mobility using Einstein equation, which is shown in Fig. 5(b). The model from [11] is widely used in the simulation software, and it is calculated by the EMC method. The model in [10] is the fitting result, which is obtained by combining the results of EMC method and experiments. The two models assume an isotropic band structure, which cannot reflect the anisotropic property of GaN [7, 25]. When the doping density becomes bigger, the simulation results of two models decrease more rapidly than our results because of the different ionized scattering model. We adopt the Brooks–Herring method, which includes the screening effect of each impurity ions Coulomb potential by the free charge carrier gas and Born scattering approximation. The model leads to larger mobility than Conwell–Weisskopf model when the carrier concentration is higher [28]. Another reason is that our method can calculate the zero-field mobility. However, the mobility obtained from velocity-electric field can only calculate the low field mobility.

In the device application, the working temperature varies from the room temperature and to satisfy this demand. We calculate the relationship between $D_l$ and temperature for the temperature range of 200 K to 600 K, which is shown in Fig. 6. It shows that the $D_l$ decreases obviously with increasing temperature. In higher temperature, electrons with higher energy are more easily scattered and lose the corre-
Damping. So, the $D_I$ becomes smaller when the temperature is higher. We can also find that the $D_I$ is larger in $\Gamma-A$ direction in the simulated temperature range.

4 Conclusions

In summary, the paper presents theoretical investigation of $D_I$ in WZ GaN as the function of electric field, frequency, doping concentration, and working temperature in $\Gamma-A$ and $\Gamma-M$ directions by the EMC technique. The results show that $D_I$ keeps constant at lower frequency. The high frequency property shows much difference for different electric field. When the electric field is lower, the $D_I$ keeps constant at first. Then it decreases with increasing frequency. However, when the electric field is larger, the $D_I$ approaches a peak value. Then it decreases with increasing frequency. The results show that $D_I$ becomes smaller at first with increasing electric field until it approaches a peak value. Then it increases with the increasing electric field, which is caused by the polar optical scattering. Finally, it decreases with increasing electric field. The $D_I$ is also impacted greatly by the ionized impurities scattering, especially when the doping concentration is higher. A comparison between our results and the references shows good agreement. The $D_I$ becomes smaller at high temperature because of stronger thermal motion of carriers. The smaller effective mass in $\Gamma-A$ direction leads to higher $D_I$ than that in $\Gamma-M$ direction in most cases.

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References