Dynamic Screened Polar Optical Phonon Scattering in Doped GaN

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Abstract

Dynamic screened scattering rate of polar optical phonons has been calculated for electrons in the central valley of GaN at moderate carrier concentrations around \(2 \times 10^{24} m^{-3}\). Our calculations used the Lindhard formalism with Fermi-Dirac distribution and with neglecting the collisional damping. Also, for simplicity nonparabolicity and the coupling between various electrons and hole have been neglected. The inverse of the dielectric function showed antiscreening peak at small phonon wave vector at carrier temperature 77 K and 300K. The screened scattering rate is strongly enhanced at low electron temperature and high carrier concentrations. This is due to antiscreening property of inverse dielectric function which appears in both emission and absorption screened optical phonons. The principle purpose of this study is too showing how the various parameters, such as carrier concentrations and carrier temperature, could change the shape of dynamic screened scattering rate of polar optical phonons.

Keywords: Screened optical phonon scattering rate, dielectric function and GaN transport

1. Introduction

In the early 1970s, interest in GaN-based devices has risen rapidly[8, 13, 15-17 ]. There has been considerable interest in GaN due to its wide band gap and
favorable material properties, such as high electron mobility and very high thermal conductivity. The large band gap energy of the III-nitrides insures that the breakdown electric field strength of these materials is much larger than that of GaAs [3, 7, 22].

It has long been known that screening of the polar interaction between electrons and optical phonons occurs dynamically rather than statistically [1-2, 14, 18-20]. Nevertheless, in most descriptions of the scattering by polar optical modes screening has been either regarded as negligible or treated statically [4-5, 18-19]. For carrier densities of $2 \times 10^2$ m$^{-3}$ and above in GaN screening becomes of considerable importance and its dynamics nature must be taken into account. Inclusion of dynamic screening has become very important, since electronic devices have been scaled down in size and scaled up doping levels.

In our model, the carrier concentrations chosen is around $2 \times 10^{24}$ m$^{-3}$, and we believe it is safe enough to ignore the electron-plasmon couple mode interaction, up to this electron concentration. Also the Pauli Exclusion Principle renders the phonon scattering rate to be negligible to simplify the calculations [1]. The Lindhard formalism [9, 21, 23] is a very good approximation to the dielectric function in the weak coupling limit.

The effect of screening was described by a renormalization of the usual effective charge $e^*$ which appears in the expression for the interaction potential. The screened effective charge is given by

$$e_s^* = e_s^* v_s (q, \omega) k_s (q, \omega)$$

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Where $v(q, \omega)$ and $v_s (q, \omega)$ are the interaction potential unscreened and screened (by free carriers) respectively and $k_s (q, \omega)$ is the high-frequency dielectric contribution from the valence band electrons.

The present paper will focus on the electron scattering by dynamically screened phonons in GaN, which will be handled at moderate carrier concentration, through the analysis of the longitudinal wave vector and frequency dependent dielectric function $k(q, \omega)$. 

2. Dynamic Screened Polar Optical Phonon Scattering Rates

The total scattering rate for screened polar optical phonon mode, can be derive as [21]

\[
W(k) = \frac{\pi}{NM} \frac{2}{\omega} \frac{c_q^2}{\delta_{k+q-k}} (n(\omega_0) + 1/2 \pm 1/2) \\
\delta(E_k' - E_k \pm h\omega_0) d^3k' 
\]

(1)

Where \( h\omega_0 \) is the longitudinal phonon energy, \( c_q^2 \) is coupling parameter which depends on the magnitude and direction of \( q \) in dynamic screened optical phonon; \( c_q^2 \) could be written as

\[
c_q^2 = \left( \frac{e^* e^*}{V \epsilon_0} \right)^2 \left( \frac{G(q, \omega)}{q} \right)^2 
\]

(2)

Where \( e^* \) is the magnitude of the effective charge on the atoms and \( V_0 \) is the volume of unit cell, \( N \) is the number of unit cell in periodic crystal and also we have defined.

\[
G(q, \omega) = k_\omega (q, \omega)/k(q, \omega) 
\]

(3)

\( M \) is the reduced mass of the two ions vibrating against each other, \( n(\omega_0) \) is the thermodynamic average number of optical phonon in equilibrium, written as

\[
n(\omega_0) = \left[ \exp\left( \frac{\hbar\omega_0}{k_B T} \right) - 1 \right]^{-1} 
\]

The upper and lower signs refer to emission and absorption of the screened polar optical phonon respectively and \( \delta_{k+q-k} \) represent momentum conservation in Umklapp scattering process. The number of final states in an elementary volume of \( q \)-space is \( V \left( \frac{2\pi}{q} \right)^3 \int d^3q \). The integral over \( k \) is equivalent to an integral over \( q \). Then Eq. (1) becomes, with \( V = NV_0 \).
Using the property of the Dirac-delta function, we obtain

\[ W(k) = \frac{V_0}{4\pi^2 \omega_0} \left( \frac{e^*}{\varepsilon_0} \right)^2 \frac{m^*}{\hbar^2 k} \left( n(\omega) \right) \int_{q_{\text{max}}}^{q_{\text{min}}} \left[ G(q, \omega) \right]^2 dq + (n(\omega) + 1) \int_{q_{\text{max}}}^{q_{\text{min}}} \frac{[G(q, \omega)]^2}{q} dq \]

Where the first term represents the screened polar optical phonon absorption while the second term corresponds to screened polar optical phonon emission. The effective charge \( e^* \) is

\[ e^* = \frac{M V_0 \omega_0^2}{2 \varepsilon_0^2 \left( \frac{1}{\varepsilon_{\infty}} - \frac{1}{\varepsilon_s} \right)} \]

Where \( \varepsilon_s \) static-frequency permittivity. Substituting \( x = \frac{q}{k_0} \) and \( dq = k_0 dx \) in Eq. (5), one obtains

\[ W(k) = \frac{e^2 \omega_0^2 m^{1/2}}{42 \sqrt{1/2} \pi \hbar \varepsilon_0} \left( \frac{1}{\varepsilon_-} - \frac{1}{\varepsilon_s} \right) \left( \frac{1}{E_k} \right)^{1/2} \left[ n(\omega) \right] \int_{x_{\text{max}}}^{x_{\text{min}}} \frac{[G(x, \omega)]^2}{x} dx + (n(\omega) + 1) \int_{x_{\text{max}}}^{x_{\text{min}}} \frac{[G(x, \omega)]^2}{x} dx \]

Where the limits of integration for both absorption and emission are

\[ x_{\text{max}} = \frac{q_{\text{max}}}{k_0} = \left( \frac{E_k}{\hbar \omega_0} \right)^{1/2} \left[ (1 \pm \frac{\hbar \omega_0}{E_k})^{1/2} + 1 \right] \]  

\[ x_{\text{min}} = \frac{q_{\text{min}}}{k_0} = \left( \frac{E_k}{\hbar \omega_0} \right)^{1/2} \left[ (1 + \frac{\hbar \omega_0}{E_k})^{1/2} - 1 \right] \]  

(absorption) 

\[ = \left( \frac{E_k}{\hbar \omega_0} \right)^{1/2} \left[ 1 - (1 - \frac{\hbar \omega_0}{E_k})^{1/2} \right] \]  

(8a) 

(8b) 

(8c)
$k(\mathbf{q}, \omega)$ written as

$$k(\mathbf{q}, \omega) = k_e(\mathbf{q}, \omega) + ik_i(\mathbf{q}, \omega)$$

The real part and imaginary part $k_R(\mathbf{q}, \omega)$ and $k_I(\mathbf{q}, \omega)$ for Fermi-Dirac distribution are obtained after using dimensionless parameter, as

$$\frac{k_R(\mathbf{q}, \omega)}{k_{\infty}(\mathbf{q}, \omega)} = \left[ 1 + \frac{3}{8} \frac{\gamma^2}{\Delta^{3/2}} \left( \frac{1}{x} \right) \int_0^\infty \frac{1}{1 + \exp \left[ \frac{1}{\theta (y^2 - \Delta_f)} \right]} \left( 1 + \frac{x}{2y} \right)^2 - \frac{1}{4x^2 y^2} \right] \left( 1 - \frac{x}{2y} \right)^2 - \frac{1}{4x^2 y^2} \right] dy$$

$$\frac{k_I(\mathbf{q}, \omega)}{k_{\infty}(\mathbf{q}, \omega)} = \frac{e \hbar q^2}{2 \pi k_B T} \left[ \left( \frac{\hbar^2 q^2}{2m} - \frac{E_f}{k_B T} \right) + \frac{E_f}{k_B T} \right]$$

We use the dimensionless variables.

$$y = \frac{\omega_p^2}{\omega} \quad \omega_p = \left( \frac{Ne^2}{\varepsilon_m} \right)^{1/2} \quad \theta = \frac{\hbar \omega}{k_B T}$$

$$y = \frac{k}{k_e} \quad x = \frac{q}{k_e} \quad k_o = \left( \frac{2m^* \omega}{\hbar} \right)^{1/2}$$

$$\Delta_i = \frac{E_i}{\hbar \omega} \quad \Delta_o = \frac{E_o}{\hbar \omega} \quad E_m = \frac{\hbar^2}{2m^*} \left( 3\pi^2 N \right)^{1/3}$$

The Fermi-Dirac distribution becomes

$$f_o(E_k) = [1 + \exp[ \theta (y^2 - \Delta_f)]]^{-1}$$
The inverse of dielectric function depends on both the wave vector \( q \) and the frequency of the phonon \( \omega \). For simplicity, we assume that \( \omega \) equals the longitudinal phonon frequency \( \omega_l \). \( E_F \) and \( E_f \) Define as Fermi energy at \( T = 0 \) and \( T_c \) respectively at carrier concentration \( N \) where \( T_c \) is the electron temperature.

3. Results and Discussion

Our aim in this section is to study the variation of screened phonon for various carrier concentrations and electron temperatures. In our study the carrier concentrations were limited below \( 2.5 \times 10^{24} \) m\(^{-3} \), at \( N=2.5\times10^{24} \) m\(^{-3} \). \( \omega_p/\omega_l = 0.6 \); therefore, the electron interaction with the collective motion of free carriers (Plasmon) is very weak. GaN parameters are taken from Foutz et al. 1999 [6], which, were originally from O’Leary et al. 2006; Lambrecht. and Segall 1994 [3, 12].

Figs.(1- a, b) represent the increase of the inverse dielectric function versus normalized phonon wave vector \( x = (q/k_0) \) for carrier concentrations \( 1 \times 10^{24} \) and \( 2 \times 10^{24} \) m\(^{-3} \) respectively, and for several values of electron temperature. The value of the inverse dielectric function increases with increasing carrier concentrations, while cooling the electron temperature also increases the inverse dielectric function value.

A comparison between emission polar optical phonon scattering rate and screened polar optical phonon scattering rate for electrons in the central valley, at a carrier concentration of \( 2 \times 10^{24} \) m\(^{-3} \) and at different electron temperatures is presented in Figs.(2- a, b) at lattice temperature of 77K and 300K respectively. We have represented both polar optical phonon scattering rates and screened polar optical phonon scattering rates by Pol and Sc respectively. It is obvious from the Figs.(2- a, b), that the Sc scattering rate is strongly enhanced at low electron temperature; this is due to antiscreening property of inverse dielectric function since for all electron energies; the antiscreening region was included in evaluating the Sc scattering rate while the screening region is very weak. As soon as the electron temperature rises, due to application high electric field, the Sc scattering rate.
becomes smaller than the Pol scattering rate at low electron energy. The Sc scattering rate is enhanced again at certain electron energy, we will call it Ec, which is defined as the electron energy at the intersection of Pol and Sc scattering rate but by small amount for low electron temperature. The value of Ec becomes larger when the electron temperature increases due to shift the antiscreening peak to large $\textbf{q}/k_0$.

As we have already mentioned, the second region of the inverse dielectric function which is the screening region appears only at both high carrier concentration and high electron temperature. Figs.(2-a, b) show the influence of both screening and antiscreening regions in the screened scattering rate, at electron temperature 77K and 300K respectively. Two regions can be observed in these figures:

1- The limits of integration of Eqs. (8a-8c) include only the screening region of the dielectric function for electron energies less than Ec, which refers to large value of $\textbf{q}/k_0$, leading to a reduction in Sc scattering rate.

2- Both screening and antiscreening regions are included in the limits of integration of Eq. (7), when the electron energy exceed Ec; this is due to a small value of $\textbf{q}/k_0$. The antiscreening peak becomes smaller at high carrier temperature, resulting in a reduction in the Sc scattering rate.

Fig. (3) presented emission Pol scattering rate and Sc scattering rate for various carrier concentration at lattice temperature and electron temperature 300K. The screened scattering rate is enhanced with increasing carrier concentrations. This emphasizes the influence of antiscreening regime.

The absorption scattering rates are very small compared to emission scattering rate especially at lattice temperature 77K, therefore, in effect, the total scattering rate represent the emission scattering rate, for both unscreened and screened cases. The polar phonon absorption scattering rate and the screened polar phonon absorption scattering rate are presented in fig. (4) for various carrier concentrations at both electron and lattice temperature 300K. This figure indicates that, the antiscreening regime has the same influence on screened optical phonon absorption scattering rate as it showed in the screened optical phonon emission scattering rate.

4. Conclusions

Dynamic screened scattering rate of polar optical phonons has been calculated for electrons in the central valley of GaN at moderate carrier concentrations.
around $3 \times 10^4 \text{m}^{-3}$. The inverse of the dielectric function showed antiscreening peak at small phonon wave vector at electron temperature 300K and carrier concentrations less than $2.5 \times 10^{24} \text{m}^{-3}$. The screened scattering rate is strongly enhanced at low electron temperature and high carrier concentrations. The influence of antiscreening peak appears in both emission and absorption screened optical phonons. This study showed how the various parameter such as carrier concentration and electron temperature could change the shape of dynamic screened scattering rate of polar optical phonons and consequently its influence on transport properties of GaN at moderate carrier concentrations.

References


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Figs. (1-a, b) Lindhard dielectric function at lattice temperature 300K versus normalized phonon wave vectors $x (q/k_0)$ for carrier concentrations $1 \times 10^{24} \text{ m}^{-3}$ and $2 \times 10^{24} \text{ m}^{-3}$ respectively, and for several values of electron temperature.
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Figs. (2-a, b) Scattering rate for polar phonon emission in the $\Gamma_1$ Valley against electron energy at different values of electron temperature.
Fig. (3) Scattering rate for polar phonon emission in the $\Gamma_1$ Valley against electron energy for various carrier concentrations.

Fig. (4) Scattering rate for polar phonon absorption in the $\Gamma_1$ Valley against electron energy for various carrier concentrations.

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