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Evaluations of the low-field mobility in degenerate GaN/AlN heterojunctions

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Abstract

We solve the linearized Boltzmann equation for a degenerate quasi-two-dimensional electron system confined to a triangular quantum well at a III nitride heterojunction and interacting only with the polar optical phonons. The method of solution makes use of a ladder technique, and employs the Fang–Howard approximation for the description of the confined electrons. The variations of the effective-momentum relaxation time with the electron energy, and of the mobility with electron density are presented for a GaN/AlN heterojunction.

The current emphasis on large-band-gap semiconductors, such as III nitrides, has necessitated the consideration of new regimes of electron transport, particularly in heterostructures. The crystal growth process often gives rise to a heterojunction in which strong intrinsic electric fields are created normal to the plane of the heterojunction. These fields are mostly strain-induced although in wurtzite materials, they can be further enhanced by contributions from spontaneous polarization [1–3]. The strong electric fields are responsible for the generation of deep potential wells which are located at the heterojunction and which act to strongly confine the electrons. As a result, two-dimensional electron densities higher than 10^{13} cm^{-2} have been observed in GaN heterojunctions even in the absence of modulation doping [4–10]. Clearly, investigations of the transport properties of such a dense electron system must incorporate the degenerate nature of the electrons. Furthermore, the potential well confining the electrons under these circumstances should be modelled as having a triangular shape which, significantly, depends on the density of the confined electrons in the manner of the well-known Fang–Howard approximation [11].

We seek to determine the solution of the Boltzmann equation in the linear regime and concentrate on the situation where there is only one electronic subband occupied since it is in the one-subband case that the quantum effects are most prominent. Our one-subband triangular quantum well model is illustrated schematically in figure 1 in which we have chosen the Fermi energy to lie below the polar optical (PO) phonon energy $\hbar\omega_{LO}$, a situation which is readily met in GaN/AlN heterojunctions, even at high densities, because of the large magnitude of the PO phonon energy ($\hbar\omega_{LO} \approx 92.8$ meV for GaN). It is well established that the dominant mechanism determining electron mobility in III nitride structures is interaction with

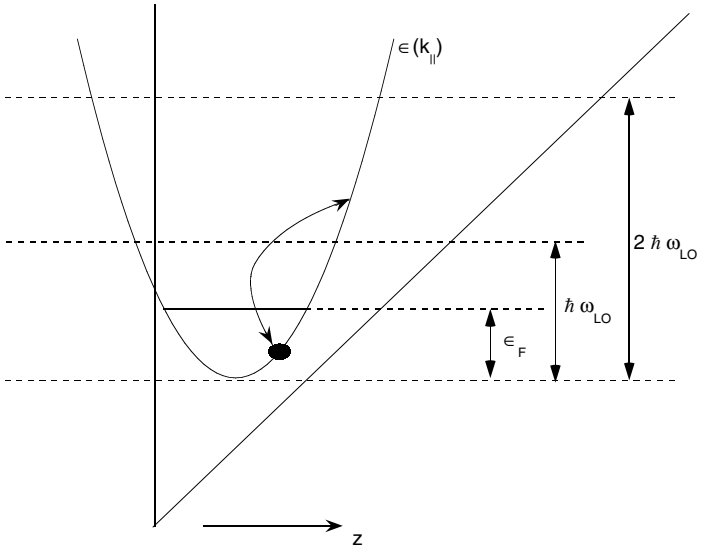

Figure 1. A schematic drawing of the one-subband model showing the lowest subband in the triangular quantum well of the heterojunction. The relative positions of the Fermi energy and two intervals of the optical phonon energy are also shown.

PO phonons. We shall assume that these PO phonons are not modified by the heterojunction and so take their bulk form [12, 13]. This is, in general, a good approximation for our purpose since we are interested in processes in which total scattering rates are sought [13]. Our first task is to calculate a momentum relaxation time, make use of the results to determine the mobility and seek to exhibit the variation of the mobility with the electron density for typical GaN/AlN heterojunctions.

The energy spectrum for electrons of effective mass m^* occupying the lowest subband is given by $\epsilon_{\boldsymbol{k}_\parallel} = \hbar^2 k_\parallel^2/2m^*$ where $\boldsymbol{k}_\parallel$ is the in-plane wavevector. The probability of transition from an electron state of in-plane wavevector $\boldsymbol{k}_\parallel$ within the lowest subband $n = 1$ to states $\boldsymbol{k}'_\parallel$ within the same subband by emission (+) or absorption (−) of a PO phonon of wavevector $\boldsymbol{q} = (\boldsymbol{q}_\parallel, q_z)$ is given by

$$W^{\pm}_{\boldsymbol{k}_\parallel,\boldsymbol{k}'_\parallel,\boldsymbol{q}} = \frac{\pi e^2 \omega_{LO}}{V_0 \varepsilon_0}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_s}\right)\left\{N + \frac{1}{2} \pm \frac{1}{2}\right\}\frac{|G(q_z)|^2}{q_\parallel^2 + q_z^2}\delta_{\boldsymbol{k}_\parallel,\boldsymbol{k}'_\parallel \pm \boldsymbol{q}_\parallel}\delta(\epsilon_{\boldsymbol{k}'_\parallel} - \epsilon_{\boldsymbol{k}_\parallel} \pm \hbar\omega_{LO}) \tag{1}$$

where $N = [\exp(\hbar\omega_{LO}/k_B T) - 1]^{-1}$ is the phonon distribution function at temperature T; e is the electronic charge, ε_s and ε_∞ are, respectively, the static and high-frequency dielectric constants of the well material (GaN), while V_0 is the large crystal volume. The function $G(q_z)$ appearing in equation (1) is appropriate for a triangular quantum well and is explicitly given by

$$G(q_z) = \frac{b^6}{(b^2 + q_z^2)^3}. \tag{2}$$

Here b is the variational parameter in the Fang–Howard wavefunction [11] and its dependence on the electron density is determined by the variational principle in the form

$$b = \left(\frac{33 e^2 m^* n_0}{8\hbar^2 \varepsilon_s \varepsilon_0}\right)^{1/3}. \tag{3}$$

We choose an average effective well width a associated with the triangular quantum well in this model as given by $a = 6/b$, which is twice the average penetration length of the charge in the GaN region [11]. Finally, in terms of $G(q_z)$, a form factor (needed later while considering the scattering and transport of electrons) is given by

$$\mathcal{F}(q_\parallel) = \int_{-\infty}^{\infty} \frac{|G(q_z)|^2}{q_\parallel^2 + q_z^2}\, \mathrm{d}q_z = \frac{\pi}{8q_\parallel}\left(1 + \frac{q_\parallel}{b}\right)^{-3}\left(8 + \frac{9q_\parallel}{b} + \frac{3q_\parallel^2}{b^2}\right). \tag{4}$$

We aim to evaluate the PO-phonon-limited low-field mobility of the degenerate 2D electron system subject to an electric field $\boldsymbol{E}$ parallel to the plane of the heterojunction. We begin by considering the linearized Boltzmann equation and seek its solution by employing a ladder technique which is described at length by Fletcher and Butcher [14] and recently used by Ridley [15]. The distribution function $f(\boldsymbol{k}_\parallel)$ of the electron system is found by solving the linearized Boltzmann equation

$$-\left(\frac{e\hbar}{m^*}\right)\boldsymbol{E}\cdot\boldsymbol{k}_\parallel\frac{\partial f_0}{\partial \epsilon} = \sum_{\boldsymbol{q}}\sum_{\boldsymbol{k}'_\parallel}\left\{W_{\boldsymbol{k}'_\parallel,\boldsymbol{k}_\parallel,\boldsymbol{q}} f(\boldsymbol{k}'_\parallel)(1 - f(\boldsymbol{k}_\parallel)) - W_{\boldsymbol{k}_\parallel,\boldsymbol{k}'_\parallel,\boldsymbol{q}} f(\boldsymbol{k}_\parallel)(1 - f(\boldsymbol{k}'_\parallel))\right\} \tag{5}$$

where f_0 is the equilibrium distribution function. The main problem when faced with this Boltzmann equation (5) is that because of the strong inelastic processes involved in the electron–PO phonon interaction, one cannot make use of the simplifying relaxation time approximation [15]. Fortunately, equation (5) can be treated as an algebraic difference equation in which the unknown energy function depends on three different arguments: $\epsilon, \epsilon + \hbar\omega_{LO}$ and $\epsilon - \hbar\omega_{LO}$. The equivalent difference equation to be solved involves an effective-momentum relaxation time $\tau(\epsilon)$ and is as follows:

$$Z\epsilon^{3/2} = A(\epsilon)\tau(\epsilon + \hbar\omega_{LO}) + B(\epsilon)\tau(\epsilon) + C(\epsilon)\tau(\epsilon - \hbar\omega_{LO}) \tag{6}$$

where Z is given by

$$Z = \frac{8\pi^2\sqrt{2}\hbar\varepsilon_0}{e^2\omega_{LO}\sqrt{m^*}}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_s}\right)^{-1} \tag{7}$$

and the coefficients A, B and C are functions of ϵ [16]. For brevity we do not quote the expressions for these coefficients here and it suffices to point out that they depend on a form factor $\mathcal{F}(q_\parallel)$ which, for the present triangular potential case, is explicitly given by equation (4).

The ladder technique [16] that we follow here involves writing equation (6) as an infinite set of equations, one for each energy interval. The set of equations is then truncated at the nth equation, and we are left to solve n equations for $(n + 1)$ unknowns. The additional condition which is needed to obtain a solution is provided by application of a boundary condition. The required additional condition is found by making use of the fact that for $\epsilon >> \hbar\omega_{LO}$ we may write $\tau(\epsilon \pm \hbar\omega_{LO}) \approx \tau(\epsilon)$, and this approximation leads to an analytical solution to equation (6) which serves as the additional condition in the system of difference equations.

Figures 2(a) and 2(b) show the variation with ϵ of the momentum relaxation time $\tau(\epsilon)$, evaluated at room temperature $T = 300$ K for a GaN/AlN single heterojunction with fixed electron density using the exact ladder method just described. The values of the electron densities in these figures are as follows: figure 2(a): $n_0 = 5.0 \times 10^{12}$ cm^{-2} and figure 2(b): $n_0 = 5.0 \times 10^{13}$ cm^{-2}. A clear feature of the result in figure 2(a) is that $\tau(\epsilon)$ exhibits steps at all integer multiples of $\hbar\omega_{LO}$. The reason behind the steps can be explained as follows. The first step arises due to the sudden onset of emission when the electron energy becomes equal to $\hbar\omega_{LO}$. The subsequent steps arise at higher multiples of $\hbar\omega_{LO}$ due to their link to the variations in the first energy interval $0 < \epsilon < \hbar\omega_{LO}$ at each absorption and emission of a phonon.

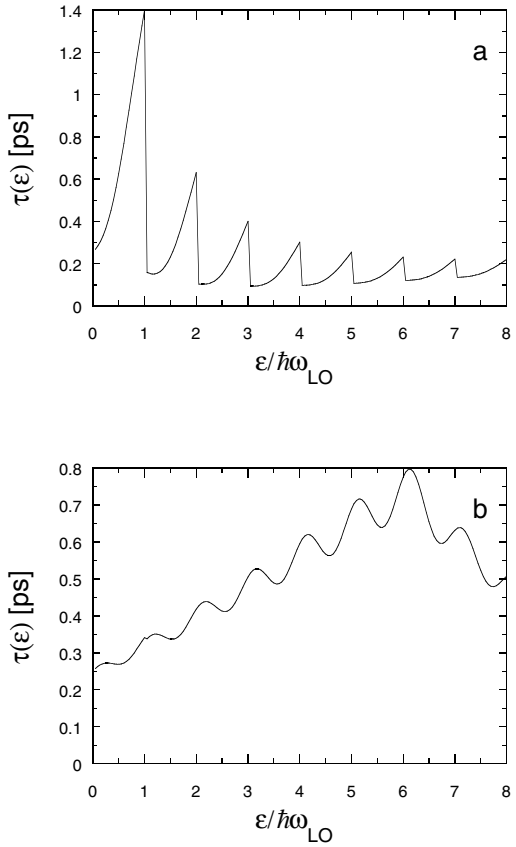

Figure 2. Variation with ϵ of the momentum relaxation time $\tau(\epsilon)$, evaluated for a fixed electron density and temperature using the exact ladder method described in the text. The values of the electron densities in these figures are as follows: (a): $n_0 = 5.0 \times 10^{12}$ cm^{-2} ($\epsilon_F = 54$ meV, $a = 5.8$ nm) and (b): $n_0 = 5.0 \times 10^{13}$ cm^{-2} ($\epsilon_F = 569$ meV, $a = 2.8$ nm). The temperature was fixed at 300 K throughout. The relevant GaN parameters are: $\hbar\omega_{LO} = 92.8$ meV; $m^* = 0.21m_e$; $\epsilon_s = 9.5$ and $\epsilon_\infty = 5.37$.

In general, τ decreases with increasing density, with smaller and less sharp steps, and the trend is such that at higher densities the steps disappear and are replaced by a smooth curve exhibiting a maximum at the Fermi energy.

The mobility μ in two dimensions is related to $\tau(\epsilon)$ as follows [17]:

$$\mu = \frac{e}{\pi\hbar^2 n_0 k_B T} \int_0^\infty \tau(\epsilon) f_0(\epsilon)[1 - f_0(\epsilon)]\epsilon \, \mathrm{d}\epsilon. \tag{8}$$

Once $\tau(\epsilon)$ has been evaluated using the ladder technique, evaluations of the mobility follow straightforwardly from equation (8) using numerical integration. The results are shown in figure 3 which shows the variations of the mobility with the electron density in a GaN/AlN heterojunction. The solid curve corresponds to the triangular quantum well and the other three to square quantum wells with different well widths [16]. It is seen that in the triangular well case the mobility decreases markedly with increasing density, while for the square wells the mobility curves are flat, except where each shows a minimum at a characteristic density. The decrease in mobility with increasing density is sharper for the triangular quantum well because of the decrease of the average effective well width with increasing density, which corresponds

to a decrease in the effective-momentum relaxation time (and hence the mobility) through the form factor. In general, the mobility is smaller when either the square quantum well width or the average effective well width for the triangular case becomes smaller. It is also interesting to note from figure 3 that the triangular and square quantum wells give similar values for the mobility when the (effective) widths match.

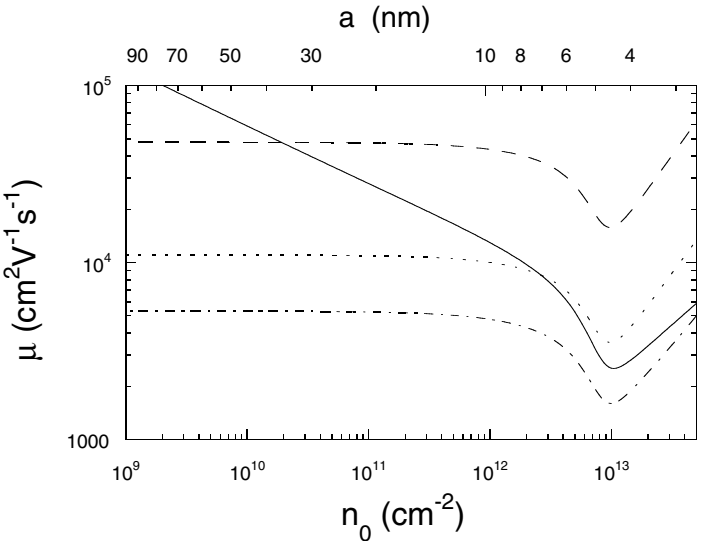

Figure 3. Variation of the mobility with the two-dimensional electron density in a single GaN/AlN heterojunction represented by a triangular quantum well (full curve). The other curves correspond to the variation of the mobility with electron density in the case of square quantum wells with different widths: 50 nm (dashed curve), 10 nm (dotted curve) and 3 nm (dot–dashed curve). The temperature is fixed at $T = 300$ K throughout and the parameters used are the same as those quoted in the caption of figure 2. The top horizontal axis shows the effective well widths of the triangular quantum well corresponding to the electron densities shown on the lower horizontal axis.

As to why each mobility curve shown in figure 3 exhibits a pronounced minimum at a characteristic density, we have checked that this feature coincides with the condition $\epsilon_F \approx \hbar\omega_{LO}$. This corresponds to an increase in the emission rate and a decrease in the momentum relaxation time. For GaN/AlN heterojunctions the drop in mobility in this region of density should, in principle, be experimentally accessible.

The theory discussed here requires further considerations involving the different regimes of approximations. In particular, screening effects, expected to come into play at high densities, must be taken into account, together with coupled-mode effects whenever the plasma frequency becomes close in magnitude to the PO phonon frequency. Furthermore, the one-subband model becomes inadequate at the densities for which the Fermi energy matches the energy separation between the lowest two subbands in the triangular well [18]. These issues will not be discussed any further here.

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