Cyclotron Mass of Electrons in GaN-$Al_xGa_{1-x}N$ Heterostructures

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The quasi-two-dimensional electron cyclotron mass in GaN-$Al_xGa_{1-x}N$ heterostructures is theoretically calculated. The shifting in Landau Levels due to the electron Longitudinal Optical phonon interaction is calculated through the Second Order Improved Wigner Brillouin Perturbation Theory (IWBPT). Experimental results recently obtained for GaN heterojunction are well described by the theory. We have also investigated the effects of the electronic density on the Cyclotron Resonance frequency.

I Introduction

Cyclotron Resonance (CR) is a powerful experimental technique to investigate the effective mass of quasi-two dimensional (Q2D) electron systems in semiconductor structures of reduced dimensionality. In the past, InSb inversion layer of the metal-oxide-semiconductor (MOS) and GaAs-AlGaAs heterostructures have been intensively studied by several authors [1]. In GaAs-based heterostructures the cyclotron resonance experiments have shown that the polaronic effects are reduced in comparison with the results for the semiconductor bulk.

More recently, the Cyclotron Resonance (CR) mass of quasi-two-dimensional electrons confined in a GaN/AlGaN heterojunction was experimentally investigated [2, 3]. Gallium Nitrite (GaN) and related III-V ternary alloys as $Al_xGa_{1-x}N$ and $Ga_xIn_{1-x}N$ are wide direct bandgap semiconductors, and the GaN is a moderately polar material with Fröhlich coupling constant $\alpha = 0.49$. Since the first report by Dingle et al.[4] on GaN optical properties numerous investigations have been made, motivated by the potential technological applications of this material for construction of the optoelectronic devices. However, little is still known about the basic properties of these materials, and only in the recent years there appeared some theoretical and experimental investigations.

In this paper we calculate the electron cyclotron mass in a GaN/AlGaN heterojunction and in a GaN Quantum Well (QW) with infinite potential barrier for the electronic confinement. We take into account the electron-phonon-longitudinal optical (LO) interaction (polaronic effects) through the Improved Wigner-Brillouin Perturbation Theory (IWBPT). The IWBPT has been successfully applied to GaAs-AlGaAs heterostructures [5 – 7]. For the GaN heterojunction our theoretical results for CR frequency were compared with the experimental results presented in Ref. [2]. We also investigate the effects of the electronic density on the CR frequency.

II Theory

The Hamiltonian describing one electron confined in the GaN side, in the heterojunction (or QW), in the presence of a magnetic field applied perpendicular to interface and interacting with the bulk LO phonons, can be written as (in the effective mass approximation),

$$H = \frac{P_z^2}{2m_b} + \frac{P_x^2}{2m_b} + \frac{m_b\omega_c^2}{2}(x - Q_y l^2) + V(z) + H_{\rm ph} + H_{\rm e-ph} \quad (1)$$

where $Q_y = \hbar P_y$, l is the classical radius of Landau, ω_c is the CR-frequency, ω_{Lo} is the LO-phonon frequency and m_b is the electron band mass. Next, the LO-phonon Hamiltonian, is given by

$$H_{\rm ph} = \hbar\omega_{Lo}\sum_{\mathbf{k}} b_{\mathbf{k}}^{+} b_{\mathbf{k}} \quad (2)$$

where $b_{\mathbf{k}}^{+}(b_{\mathbf{k}})$ is the creation (annihilation) operator for the bulk LO phonon of wave vector $\mathbf{k} = (\mathbf{K}, \mathbf{k}_z)$. The electron–LO-phonon interaction is described by the Fröhlich Hamiltonian

$$H_{e-ph} = \sum_{\mathbf{k}} (V_k e^{i\mathbf{k}\cdot\mathbf{r}} b_{\mathbf{k}} + V_k^{*} e^{-i\mathbf{k}\cdot\mathbf{r}} b_{\mathbf{k}}^{+}), \quad (3)$$

where

$$V_k = -\frac{i\hbar\omega_{Lo}}{|\mathbf{k}|}\left(\frac{4\pi\alpha}{V}\right)^{1/2}, \quad (4)$$

and α and V are the standard coupling constant for GaN and the volume of the system, respectively. The electron-phonon interaction shifts the Landau energy level. In this way we have that the dimensionless polaron energy is given by,

$$E_n = (n + \frac{1}{2})\lambda^2 + \Delta E_n \quad (5)$$

where $\lambda^2 = \frac{\omega_c}{\omega_{Lo}}$ and the energy correction, ΔE_n , is calculated through the second order Improved Wigner Brillouin Perturbation Theory (IWBPT) yielding the correct pinning behavior for coupling constant $\alpha < 1$. The IWBPT, as well the memory function formalism [8], has been successfully applied to GaAs/AlGaAs heterostructures. Therefore ΔE_n is given by

$$\Delta E_n = -\alpha \sum_{m=0}^{\infty} \frac{n_2!}{n_1!} \int_0^{\infty} \frac{F(q) L_{n_2}^{n_1-n_2}(q^2/\lambda^2)}{1 - \Delta_n - W_{nm}} e^{\frac{-q^2}{\lambda^2}} \left(\frac{q^2}{\lambda^2}\right)^{n_1-n_2} dq \quad (6)$$

where the parameters $n_1$and n_2 denotes respectively the maxima and the minima between the indices n and m. $L_{n_2}^{n_1-n_2}(x)$ is the associate Laguerre polynomial and $W_{nm} = (n-m)\lambda^2$ is the parabolic energy transition between the Landau levels n and m . In the IWBPT , $\Delta_n = \Delta E_n - \Delta E_o^{RSPT}$, where ΔE_o^{RSPT} is obtained through the Rayleigh-Schrödinger Perturbation Theory (RSPT). The form factor, taking into account the dimensionality of the system, is given by,

$$F(q) = \int dz \int dz' |\phi(z)|^2 |\phi(z')|^2 \exp(-q|z - z'|) \quad (7)$$

where $\phi(z)$ is the electron wave function in the z-direction, and we have used the Fang-Howard wave function [5, 6, 7] for the heterojunction. For the one-dimension QW having width L and the potential barrier having infinite height, we use the standard wave function for an electron confined in this system.

The CR mass as a function of the electron band mass is obtained by evaluating numerically the expression

$$\frac{m^*}{m_b} = \left(1 + \frac{\Delta E_1 - \Delta E_0}{\lambda^2}\right)^{-1} \quad (8)$$

as a function of the magnetic field strength. The effective CR-frequency is connected with the CR effective mass by the relation:

$$\omega_c^* = \frac{\lambda^2}{(m^*/m_b)}\omega_{Lo}. \quad (9)$$

III Results and Discussions

In this section we present the theoretical results obtained for GaN heterostructures. The values of physical GaN parameters used in the calculation were: $\hbar\omega_{Lo} = 92meV$, $Eg = 3.5eV$, $\alpha = 0.49$ and the electron band

mass was treated as a fitting parameter, to be determined by comparison of experimental data [2] with our theoretical results.

In Fig. 1 we have shown the CR-frequency as a function of the applied magnetic field, for a GaN/AlGaN heterojunction with electronic density $N_s = 3.1 \cdot 10^{12} cm^{-2}$. The experimental results shown in this figure (circles with error barrs) were obtained by Knap and co-workers [2]. Our theoretical results (solid line) were calculated for the electron band mass assumed as $m_b = 0.223 m_e$, where m_e is the free electron mass. We can note a good agreement between both the experimental and theoretical results. The qualitative behavior of the CR-frequency as function of the applied magnetic field is the same as observed previously for heterostructures of GaAs [5 – 8]. However, in GaAs structures the effects of non parabolicity of the conduction band and the screening of the electron-phonon interaction are decisive for the fitting of the experimental data [5 – 8]. Here we have neglected these effects because, for the available set of experimental data, the inclusion of these effects do not improve the agreement between the experimental and theoretical results. The results by Knap et al. [2] for the electron band mass at the bottom of the conduction band were $m_b = (0.223 \pm 0.011) m_e$ which agrees with our best fit of the experimental data shown in the Fig. 1. Other experimental values found in the literature for m_b/m_e are 0.219 [3], 0.220 ± 0.005 [9] and 0.21 ± 0.02 [10].

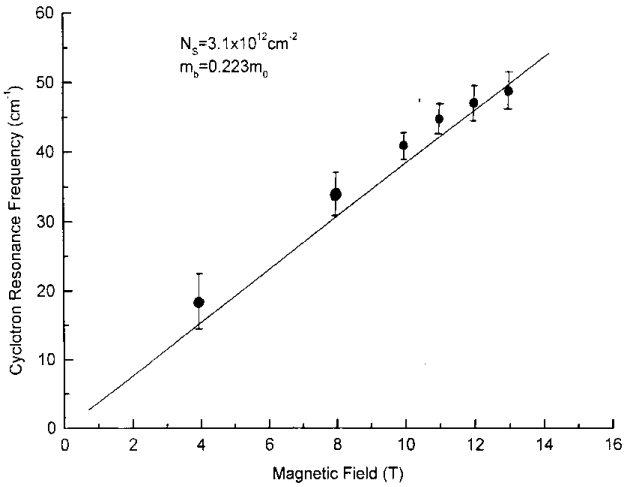

Figure 1. CR frequency as a function of the applied magnetic field, for a GaN heterojunction with electronic density $N_s = 3.1 \cdot 10^{12} cm^{-2}$. The experimental results shown in the figure are those by Knap and co-workers [2] and our theoretical results (solid line) came from the electron band mass assumed as $m_b = 0.223 m_e$.

Recently, Wu and Peeters [11] calculated the correction to the electron CR mass using the memory function formalism. As the IWBPT, this formalism has been successfully applied to GaAs-based heterostructures over the whole magnetic field range [7]. The electron band mass was assumed as $m_b = 0.22 m_e$ and a good agreement between the experimental data and the theoretical curves was observed. This calculation has taken into account the non parabolicity of the conduction band and the screening of the electron-phonon interaction.

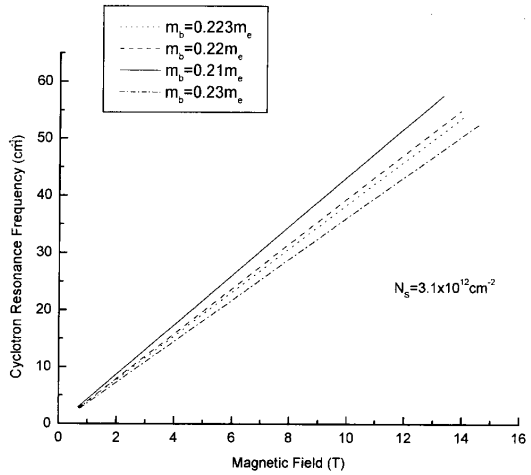

Figure 2. The magnetic field dependence of the CR frequency for a GaN heterojunction with electronic density $N_s = 3.1 \cdot 10^{12} cm^{-2}$, for various electron band mass values.

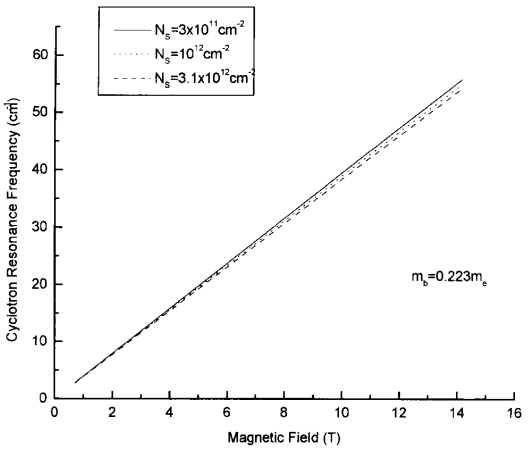

Figure 3. Theoretical results for the CR frequency calculated for three values of the electronic density, $3.1 \cdot 10^{11} cm^{-2}$, $10^{12} cm^{-2}$and $3.1 \cdot 10^{12} cm^{-2}$, the electron band mass being assumed as $m_b = 0.223 m_e$.

In Fig. 2, the magnetic field dependence of the CR frequency is shown for four values of the electron band mass. As we can observe the CR-frequency is very sensitive to a small variation in the electron band mass and as the magnetic field increases the differences between the results for different values of m_b increases. Fig.3 shows the CR frequency as a function of the magnetic field, for three electronic densities. The CR frequency

decreases as the electronic densities increase, this being due to the narrowing of the electronic layer, which increases the CR mass via the form factor given in the Eq.(7).

Fig. 4 shows the CR mass of electrons confined in a GaN quantum well with infinite height for the potential barrier, as a function of the applied magnetic field (solid lines). Also, for comparison, we have plotted in this figure the results for a GaN/AlGaN heterojunction (dotted lines).The qualitative behavior of the curves are the same observed previously for GaAs-structures [4−6, 8]. Note in this figure that the width of the electronic layer in the heterojunction is approximately $35\mathring{A}$, corresponding to an electronic density $N_s = 3.1 \cdot 10^{12} cm^{-2}$, while for the QW the width is $L = 100\mathring{A}$. Also, we can observe that, below the resonance ($\omega_c < \omega_{LO}$) the CR mass is higher for the heterojunction than for QW due to the highest confinement the reverse occurring above the resonance.

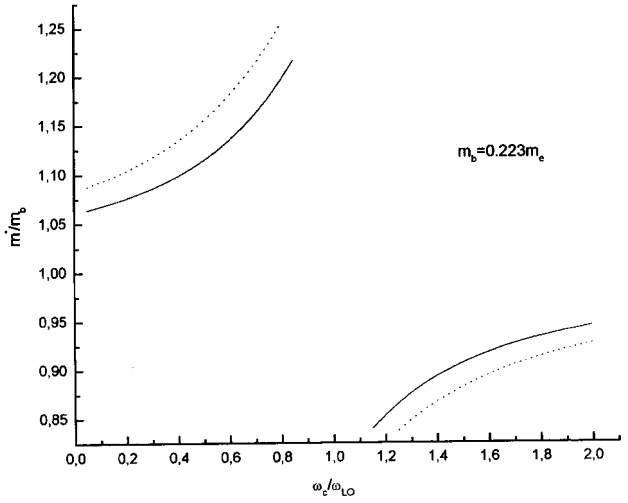

Figure 4. Electron CR mass as function of the applied magnetic field for two GaN heterostructures, a quantum well with infinite height for the potential barrier (solid lines) and a heterojunction (dotted line). The parameters used in the calculations were, $m_b = 0.223 m_e$, $N_s = 3.1 \cdot 10^{12} cm^{-2}$ and $L = 100\mathring{A}$.

As a résumé, we have made a calculation of the CR frequency (and mass) of electrons confined in GaN heterostructures including the electron-LO phonon interaction. For GaN/AlGaN heterojunction we compare our theoretical results with recent experimental data and a good agreement is found when the electron effective mass is taken as $m_b = 0.223 m_e$. Theoretical results for the electron CR mass in a GaN quantum well (infinite confinement) are considered.

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