The magnitude of the conduction band non-parabolicity (NP) in wurtzite GaN currently remains controversial. NP of a band can be probed by measuring the carrier effective mass \(m^*\) as a function of energy. Such experiments have been performed in the past in both bulk and in two-dimensional electron systems (2DES). The deduced band edge mass values, \(m_0^*\), however, exhibit considerable scatter. Using cyclotron resonance (CR), Drechsler et al. \[6\] determined \(m_0^*\) in bulk wurtzite GaN to be 0.20\(m_e\), where \(m_e\) is the free electron mass. Other methods such as infrared reflectivity on electron plasma \[2\] and spectroscopy on shallow donors \[3, 4, 5\] in bulk GaN have yielded 0.220\(m_e\) < \(m_0^*\) < 0.236\(m_e\). An even wider range of values for the band edge mass, 0.185\(m_e\) < \(m_0^*\) < 0.231\(m_e\), emerge from experiments in AlGaN/GaN heterostructures. From the temperature dependence of Shubnikov-de Haas (SdH) oscillations of 2DES, Lin et al. deduced \(m_0^* = 0.22m_e\) \[6\] while Hang et al. reported \(m_0^* = 0.185m_e\) \[7\]. Cyclotron resonance experiments on heterostructures have revealed 0.223\(m_e\) < \(m_0^*\) < 0.231\(m_e\) \[8, 9\]. This spread in \(m_0^*\) suggests that the “extrapolation” from the various experiment values \(m^*(E)\) to the band edge remains poorly controlled.

Using CR we have measured \(m^*\) in a series of high mobility (∼20,000 cm²/V·sec) AlGaN/GaN structures. Our heterostructures are all grown by molecular beam epitaxy (MBE) on GaN templates prepared by hydride vapor phase epitaxy (HVPE). The specimens are described in detail elsewhere \[10, 11\]. Our data cover a density range of \(1 − 6 × 10^{12} \text{ cm}^{-2}\). In these 2D systems this implies energies from ∼27meV to ∼120meV above the band edge due to electron confinement and band filling. Therefore, our mass data probe the NP of the GaN conduction band in small steps over a wide energy range. We also perform extensive \(k.p\) calculations and determine that instead of the commonly used two-band model, a multi-band model is required to explain our experimental results. Additionally, our calculations on polaron correction of the effective mass of 2D electrons in GaN show them to be at the 1% level, considerably less than previously thought \[8\]. A detailed comparison between our data and \(k.p\) calculation sets the band mass value to \(m_0^* = (0.208 ± 0.002)\(m_e\) and, when applied to other investigators’ results, considerably reduces the spread in band edge mass values.

A Fourier transform spectrometer with light pipe optics and a composite Si bolometer was used for the detection of far-infrared transmission. Magnetic field was applied normal to the 2D electron layer. The carrier density of each sample was determined in situ from the Shubnikov-de Haas (SdH) oscillations of the 2DES. All CR and SdH experiments were conducted at 4.2K.

Fig. 4 shows the cyclotron resonance energies versus magnetic field, \(B\), of a sample with \(n_{2D} = 2.3 × 10^{12} \text{ cm}^{-2}\). All data are taken with a resolution of 0.24 meV. The inset shows high field transmission spectra normalized to the spectrum taken at \(B=0\)T. The solid line in Fig.1 is a fit to the data at high fields, \(B>27\)T, and low fields, \(B<12\)T, resulting in an effective mass of \(m^* = 0.228m_e\). For 15T>B<25T, there is a pronounced deviation from this straight line. This anomaly in the CR represents a recent discovery, which is being analyzed and published elsewhere \[12\]. Here, we observe that this anomaly is limited to a finite field region outside which all CR data can be fit by a straight line.

We have measured the effective mass in eleven samples with carrier density, \(n_{2D}\), ranging from \(1 − 6 × 10^{12} \text{ cm}^{-2}\). In all cases, we observed either a broadening or a splitting of the CR line at intermediate fields but could fit the data away from this regime as well as the data seen in Fig. 4.
FIG. 1: Resonance energies vs. $B$ of a sample with $n_{2D} = 2.3 \times 10^{12}$ cm$^{-2}$. High and low field resonances can be fit with a single straight line, giving an effective mass of $0.228 m_e$. Near 18T a level anti-crossing results in a splitting of the CR (see text). Inset: Transmission data for $B=26$, 28, and 30T, normalized to the spectrum at $B=0T$.

Fig. 2 shows the dependence of $m^*$ on $n_{2D}$. For comparison, we also plot data from Ref. $[8,9,12]$. The mass data from the different references are located in the general vicinity of our results but, due to their considerable error bar or sparsity, are difficult to extrapolate to zero density. The combined data of Fig. 2 show an increase in $m^*$ by $\sim 17\%$ as $n_{2D}$ changes from $1 - 9 \times 10^{12}$ cm$^{-2}$. The rise in $m^*$ with $n_{2D}$ reflects the non-parabolicity of the conduction band of the GaN host. Simply extrapolating our closely spaced data linearly to vanishing $n_{2D}$, we arrive at $m^*_0 = 0.214 m_e$. This value is about $\sim 8\%$ lower than previously published CR data $[8,12]$. Since our data contain a small error bar and extend to very low $n_{2D}$, such a simple extrapolation should already be quite reliable.

Other groups have previously addressed NP in GaN. For example, Knap et al. explored NP using CR with different $n_{2D}$ (see our Fig. 2) and accounted for the magnitude of NP using a simple two-band approximation $[8,12]$. In such an approximation, which includes only coupling between the lowest conduction and highest valence bands, the effective mass varies as

$$m^*(E) = m^*_0 (1 + 2KE/E_g)$$

(1)

with $K=1$ and $E_g=3.5$ eV. In a 2DES the energy, $E = E_k + E_F$, above the band minimum is composed of the average kinetic energy, $E_k$, of the electrons in the confining potential well and $E_F = \pi \hbar^2 n_{2D}/m^*_0 [13]$, the Fermi energy of the 2D electron system. The value of $E_k$ is dependent on the form of the wave function of the confined electrons. In a simple triangular potential approximation, the average kinetic energy is $E_k = E_c/3$, with $E_c$ being the confinement energy of the lowest subband $[14]$. Using the more accurate Fang-Howard variational wave function gives $E_k = \hbar^2 b^2 / 8m^*_0$, where $b^2 = 48 \pi m^*_0 e^2 (N_{dep} + \frac{11}{3} n_{2D}) / e^2 [14]$. In our samples, since both the MBE and the HVPE GaN are n-type, the depletion layer density, $N_{dep}$, can be set to zero. We use this two-band model with only one adjustable parameter, $m^*_0$, to fit the high-density data of Ref. [8] (dashed line in Fig. 2). $E_k$ was computed in the triangular approximation following the authors of Ref. [8]. Clearly, although this procedure can describe the original density dependence of $m^*$ of Ref. [8] due to the rather large error bars, it fails to account for our data. Neither a simple vertical shift of the line (a different $m^*_0$) nor the usage of the Fang-Howard wavefunction can resolve this discrepancy. What is required, is a much stronger dependence of $m^*$ on $n_{2D}$.

Empirically, we pursue an approach taken by Singleton et al. $[14]$, who used a modified two-band model to describe their NP data in GaAs. The authors considered $K$ in Eq. (1) to be a second fitting parameter. The inclusion of a variable $K > 1$ into the analytic expression incorporates the influence of higher conduction bands, simulating the results of a more elaborate, multi-band calculation $[14]$. Working with the Fang-Howard model to determine $E_k$ we find a very good fit to our data for $K = 2.5$ and $m^*_0 = (0.208 \pm 0.002) m_e$. Even if we use the less reliable triangular approximation, the required $K = 1.9$. The effectiveness of the modified expression in fitting
the density dependence of \( m^* \) over a wide range of \( n_{2D} \) demonstrates that the conduction band of GaN is more non-parabolic than was previously assumed \[2\] .

Before concluding that the proposed NP model appropriately describes our CR data, we need to assure ourselves that polaron effects are a negligible contributor to \( m^* \). This mass enhancement factor results from electron-LO phonon coupling in polar semiconductors, such as GaN. A determination of a polaron mass enhancement in heterostructures requires inclusion of screening in 2D and the finite width of the electronic wave function \[17\], since both greatly reduce interaction between 2D carriers and LO phonons \[18\]. Following Ref. \[18\], we calculated the polaron effective mass in AlGaN/GaN heterostructures using a a Frohlich constant, \( \alpha = 0.49 \) \[1\]. Fang-Howard variational wave function, and a static Thomas-Fermi screening model. We find a polaron enhancement of less than 1% for \( n_{2D} = 3.1 \times 10^{12} \text{cm}^{-2} \). Since the effect decreases with decreasing density, corrections for lower density specimens are smaller yet. This mass enhancement is considerably smaller than the 10% estimated previously for \( n_{2D} = 9 \times 10^{12} \text{cm}^{-2} \) \[3\]. Following Ref. \[18\], we calculated the polaron effective mass in AlGaN/GaN heterostructures using a Frohlich constant, \( \alpha = 0.49 \) \[1\]. Fang-Howard variational wave function, and a static Thomas-Fermi screening model. We find a polaron enhancement of less than 1% for \( n_{2D} = 3.1 \times 10^{12} \text{cm}^{-2} \). Since the effect decreases with decreasing density, corrections for lower density specimens are smaller yet. This mass enhancement is considerably smaller than the 10% estimated previously for \( n_{2D} = 9 \times 10^{12} \text{cm}^{-2} \).

The large spread in the value of the band edge mass \( m_0^* \) in the literature is mostly due to two reasons: the underestimation of the NP and the overestimation of polaronic corrections. Applying our NP and polaron corrections to the available effective mass data (Ref. \[1 \[2\] \[3\] \[4\] \[5\] \[6\] \[7\] \[8\] \[9\] \[10\] \[11\] \[12\] \[13\] \[14\] \[15\] \[16\] \[17\]), we reach a much more coherent picture for the band edge effective mass, \( m_0^* \), in GaN, as shown in the inset to Fig. 2. We observe that the majority of the values for \( m_0^* \) are very close to an average \( m_0^* = 0.204 m_e \). However, most of the \( m_0^* \) data from SdH (displayed in stars) remain at variance from the CR, infra-red reflectivity and donor spectroscopy data, a fact that remains unexplained.

Since \( m^*(E) \) cannot be accurately represented with a two-band model, a five-band \( k.p \) calculation \[16\] in the zincblende approximation was performed to model our data. Figure 3 shows the results. The material parameters employed using the Koster notation are the spin-orbit splitting, \( \Delta_0 ' \), of the \( \Gamma_5 \) conduction band and the momentum matrix elements, \( P^2 \) and \( \lambda^2 P^2 \), coupling the \( \Gamma_1 \) conduction band with the \( \Gamma_5 \) valence and conduction bands. They are not precisely known. The formalism proposed by Carlos et al. \[18\] and used by Bayerl et al. \[20\] in a 5-band model to relate the parameters was utilized to calculate \( m^*(E) \). However, as seen in Fig. 3, the parameters chosen by Bayerl et al. lead to a non-parabolicity even lower than in a two-level model. We find that the experimental data points can only be matched if an extra parameter \( C \), taking remote bands into account at \( k=0 \), is included \[21\]. If one assumes \( C = -1.5 \) (compare with \( C = -2 \) for GaAs \[10\]), \( P^2 \) is in the range 25-27 eV with \( \lambda^2 \approx 0.33-0.48 \) and \( \Delta_0 ' \approx 120-180 \) meV. This set of parameters is close to the “best” set of values chosen by Kennedy et al. \[22\] and confirm that \( P^2 \) is relatively large for GaN (\( P^2 \approx 26 \) eV).

In conclusion, our CR experiments set the conduction band edge mass in GaN to \( m_0^* = (0.208 \pm 0.002) m_e \). Using our determination of the nonparabolicity and reviewing the polaron correction we reach much better agreement between several published data for \( m_0^* \).

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**FIG. 3:** Variation of \( m^* \) with energy according to \( k.p \) calculations, assuming \( m_0^* = 0.208 m_e \). The two-band model and the five-band \( k.p \) results of Bayerl et al., which neglect remote bands both underestimate the energy-dependence of \( m^* \). The experimental data (solid squares) can be explained by multiband \( k.p \) calculations that include the influence of remote bands (dashed lines).
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