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Nonparabolicity of the conduction band of wurtzite GaN

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Using cyclotron resonance, we measure the effective mass, m^*, of electrons in AlGaN/GaN heterostructures with densities, $n_{2D} \sim 1$ to 6×10^{12} cm^{-2}. From our extensive data, we extrapolate a band edge mass of $(0.208\pm0.002)m_e$. By comparing our m^* data with the results of a multiband $\mathbf{k}\cdot\mathbf{p}$ calculation, we infer that the effect of remote bands is essential in explaining the observed conduction-band nonparabolicity (NP). Our calculation of polaron mass corrections—including finite width and two-dimensional (2D) screening—suggests those to be negligible. It implies that the behavior of $m^*(n_{2D})$ can be understood solely in terms of NP. Finally, using our NP and polaron corrections, we are able to reduce the large scatter in the published band edge mass values. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1630369]

The magnitude of the nonparabolicity (NP) of the conduction band of wurtzite GaN currently remains controversial. NP of a band can be probed by measuring the 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.*[1] determined m_0^* in bulk wurtzite GaN to be $0.20m_e$, where m_e is the free electron mass. Other methods, such as infrared reflectivity on electron plasma[2] and spectroscopy on shallow donors[3–5] in bulk GaN have yielded $0.220m_e < m_0^* < 0.236m_e$. An even wider range of values for the band edge mass, $0.185m_e < m_0^* < 0.231m_e$, emerge from experiments in AlGaN/GaN heterostructures. From the temperature dependence of Shubnikov-de Haas (SdH) oscillations of 2DES, Lin *et al.*[6] deduced $m_0^* = 0.22m_e$ while Hang *et al.*[7] reported $m_0^* = 0.185m_e$. CR experiments on heterostructures have revealed $0.223m_e < m_0^* < 0.231m_e$.[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 ($\mu \sim 20\,000$ cm^2/V s) 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 from 1 to 6 $\times10^{12}$ cm^{-2}. In these two-dimensional (2D) systems, this implies energies from ~27 meV to ~120 meV 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 $\mathbf{k}\cdot\mathbf{p}$ calculations and determine that instead of the commonly used two-band model a multiband 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 $\mathbf{k}\cdot\mathbf{p}$ calculation sets the band mass value to $m_0^* = (0.208\pm0.002)m_e$ and, when applied to the results of other investigators, 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. A magnetic field was applied normal to the 2D electron layer. The carrier density of each sample was determined *in situ* from the SdH oscillations of the 2DES. All CR and SdH experiments were conducted at 4.2 K.

Figure 1 shows the CR energies versus magnetic field, B of a sample with $n_{2D} = 2.3\times10^{12}$ cm^{-2}. All data are taken with a resolution of 0.24 meV. The inset of Fig. 1 shows high-field 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 15 T $< B <$ 25 T, there is

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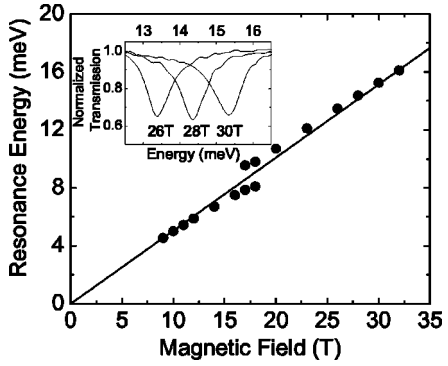

FIG. 1. Resonance energies vs magnetic field, B, of a sample with $n_{2D}=2.3\times10^{12}$ cm^{-2} taken with a resolution of 0.24 meV. High- ($B>27$ T) and low-($B<12$ T) field resonances can be fit with a single straight line, giving an effective mass of $0.228m_e$. Near 18 T, a level anticrossing results in a splitting of the CR. Inset: Transmission data for $B=26$, 28, and 30 T, normalized to the spectrum at $B=0$ T.

a pronounced deviation from this straight line. This anomaly in the CR is being analyzed and published elsewhere.[10] 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 11 samples with carrier density, n_{2D}, ranging from 1 to 6×10^{12} 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. 1. Figure 2 shows the dependence of m^* on n_{2D}. For comparison, we also plot data from Refs. 8, 9, and 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, i.e., to the conduction-band minimum. The combined data of Fig. 2 show an increase in m^* by $\sim$17% as n_{2D} changes from 1 to 9×10^{12} cm^{-2}. The rise in m^* with n_{2D} reflects the NP of the conduction band of the GaN host. Simply extrapolating our closely spaced data linearly to vanishing n_{2D}, we arrive at a band edge mass of $m_0^*=0.214m_e$. This value is about

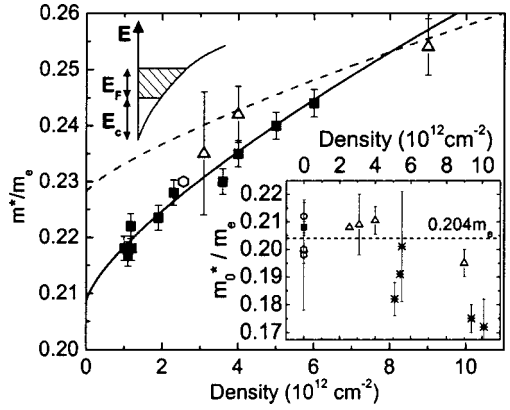

FIG. 2. Effective mass, m^*, in AlGaN/GaN systems vs 2D electron density. Our data are shown as solid squares. Data from Refs. 8, 9, and 12 are shown as open symbols. The dashed line is a two band fit to the results of Ref. 9 according to Eq. (1) with $K=1$. The solid line represents a fit with $K=2.5$, which accounts for the influence of additional, higher conduction bands. Inset: Values of the band edge, mass from Refs. 1–9, 12, and this work, after NP and polaron corrections. CR results are shown as open triangles, donor spectroscopy data as open hexagons and SdH data as stars. Our result of $m_0^*=(0.208\pm0.002)m_e$ is shown as a solid square. Averaging all data (except SdH) yields $m_0^*=0.204m_e$ illustrated by a dashed line.

$\sim$8% lower than previously published CR data.[8,9] 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.*[8,9] explored NP using CR in AlGaN/GaN systems with different n_{2D} (see Fig. 2) and accounted for the magnitude of NP using a simple two-band approximation. In such an approximation, which includes only coupling between the lowest conduction and highest valence bands, the effective mass varies as

$$m^*(E)=m_0^*(1+2KE/E_g), \tag{1}$$

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 $E_F=\hbar^2\pi n_{2D}/m_0^*$,[13] the Fermi energy of the 2DES. 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 measured from the bottom of the conduction band.[14] Using the more accurate Fang–Howard variational wave function gives $E_k=\hbar^2b^2/8\,m_0^*$, where $b^3=48\pi m_0^*e^2(N_{dep}+11/32n_{2D})/\epsilon\hbar^2$.[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. 9 (dashed line in Fig. 2). E_k was computed in the triangular approximation following the authors of Ref. 9. Clearly, although this procedure can describe the original density dependence of m^* of Ref. 9 due to the rather large error bars, it fails to account for our own data. Neither a simple vertical shift of the line (a different m_0^*) nor the usage of the Fang–Howard wave function 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.*,[15] 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, multiband $\mathbf{k}\cdot\mathbf{p}$ calculation.[16] Working with the Fang–Howard model to determine E_k, we find a very good fit to our data for $K=2.5$ and $m_0^*=(0.208\pm0.002)m_e$. 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 nonparabolic than was previously assumed.[6–9]

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–longitudinal optical (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 Fang–

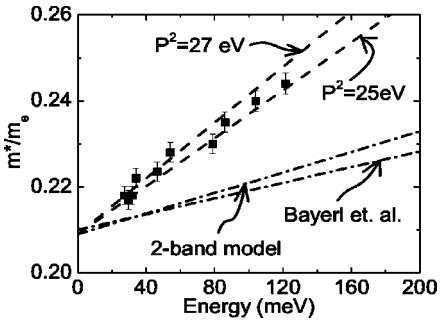

FIG. 3. Variation of m^* with energy according to $\mathbf{k}\cdot\mathbf{p}$ calculations, assuming a band edge mass of $0.208m_e$. The two-band model and the five-band $\mathbf{k}\cdot\mathbf{p}$ results of Bayerl *et al.* (see Ref. 20), which neglect remote bands, both underestimate the energy dependence of m^*. The experimental data (solid squares) can be explained by multiband $\mathbf{k}\cdot\mathbf{p}$ calculations, that include the influence of remote bands.

Howard variational wave function, a static Thomas–Fermi screening model, and a Frohlich constant, $\alpha=0.49$.[1] We find a polaron enhancement of less than 1% for m^* for $n_{2D}=9\times10^{12}$ 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 $n_{2D}=3.1\times10^{12}$ cm^{-2}, where screening and finite width had been neglected.[8] A 1% mass enhancement, due to polaronic coupling, lies within the error bars of our CR data.

The large spread in the value of the band edge mass m_0^* in 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 (Refs. 1–9 and 12), 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 $m_0^*=0.204m_e$. However, most of the m^* data from SdH (displayed in stars in Fig. 2) remain at variance from the CR, infrared 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 $\mathbf{k}\cdot\mathbf{p}$ 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, Δ_0', of the Γ_5 conduction band and the momentum matrix elements, P^2 and λ^2P^2, coupling the Γ_1 conduction band with the Γ_5 valence and conduction bands. They are not precisely known. The formalism proposed by Carlos *et al.*[19] and used by Bayerl *et al.*[20] in a five-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.*[20] lead to an NP 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 at $k=0$ into account, is included.[21] If one assumes $C=-1.5$ (compare with $C=-2$ for GaAs),[16] P^2 is in the range 25–27 eV with $\lambda^2\approx0.33-0.48$ and $\Delta_0'\approx120-180$ meV. This set of parameters is close to a good set of values chosen by Kennedy[22] and confirm that P^2 is relatively large for GaN ($P^2\approx26$ eV).

In conclusion, our CR experiments set the conduction band edge mass in GaN to $m_0^*=0.208\pm0.002m_e$. Using our determination of the NP and reviewing the polaron correction, we reach much better agreement between several published data for m_0^*.

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[1] M. Drechsler, D. M. Hofmann, B. K. Meyer, T. Detchprohm, H. Amano, and I. Asasaki, Jpn. J. Appl. Phys., Part 1 **34**, L1178 (1995).
[2] P. Perlin, E. Litwin-Staszewska, B. Suchanek, W. Knap, J. Camassel, T. Suski, R. Piotrzkowski, I. Grzegory, S. Porowski, E. Kaminska, and J. C. Chervin, Appl. Phys. Lett. **68**, 1114 (1996).
[3] W. J. Moore, J. A. Freitas, Jr., and R. J. Molnar, Phys. Rev. B **56**, 12073 (1997).
[4] A. M. Witowski, K. Pakula, J. M. Baranowski, M. L. Sadowski, and P. Wyder, Appl. Phys. Lett. **75**, 4154 (1999).
[5] B. K. Meyer, D. Vohm, A. Graber, H. C. Alt, T. Detchprohm, A. Amano, and I. Akasaki, Solid State Commun. **95**, 597 (1995).
[6] T. Y. Lin, H. M. Chen, M. S. Tsai, Y. F. Chen, F. F. Fang, C. F. Lin, and G. C. Chi, Phys. Rev. B **58**, 13793 (1998).
[7] D. R. Hang, C.-T. Liang, C. F. Huang, Y. H. Chang, Y. F. Chen, H. X. Jiang, and J. Y. Lin, Appl. Phys. Lett. **79**, 66 (2001).
[8] W. Knap, S. Contreas, H. Alause, C. Skierbiszewski, J. Camassel, M. Dyakonov, J. Yang, M. Asif Khan, Q. Chen, J. Yang, M. L. Sadowski, S. Huant, F. H. Yang, M. Goiran, J. Leotin, and M. S. Shur, Appl. Phys. Lett. **70**, 2123 (1997).
[9] W. Knap, H. Alause, J. M. Bluet, J. Camassel, J. Young, M. Asif Khan, Q. Chen, S. Huant, and M. Shur, Solid State Commun. **99**, 195 (1996).
[10] S. Syed, M. J. Manfra, Y. J. Wang, H. L. Stormer, and R. J. Molnar, Phys. Rev. B **67**, 241304 (2003).
[11] M. J. Manfra, N. G. Weimann, J. W. P. Hsu, L. N. Pfeiffer, K. W. West, S. Syed, H. L. Stormer, W. Pan, D. V. Lang, S. N. G. Chu, G. Kowach, A. M. Sergent, J. Caissie, K. M. Molvar, L. J. Mahoney, and R. J. Molnar, J. Appl. Phys. **92**, 338 (2002).
[12] Y. J. Wang, R. Kaplan, H. K. Ng, K. Doverspike, D. K. Gaskill, T. Ikedo, I. Akasaki, and H. Amono, J. Appl. Phys. **79**, 8007 (1996).
[13] Here we use an average mass of $m_0^*=0.23m_e$, since it enters E_F as $(m_0^*)^{-1}$ and E_k as $(m_0^*)^{-1/3}$ and therefore enters m^* in higher order.
[14] T. Ando, F. B. Fowler, and F. Stern, Rev. Mod. Phys. **54**, 437 (1982).
[15] J. Singleton, R. J. Nicholas, D. C. Rogers, and C. T. B. Foxon, Surf. Sci. **196**, 429 (1988).
[16] P. Pfeffer and W. Zawadzki, Phys. Rev. B **41**, 1561 (1990).
[17] According to S. Das Sarma, Phys. Rev. B **27**, 2590 (1983); phase-space restrictions due to the degeneracy of the 2DES can be ignored for k_F/q_0 at least as high as 0.6, where q_0 is the phonon wave vector. In our AlGaN/GaN systems $k_F/q_0\leqslant0.6$ for $n_{2D}\leqslant3.4\times10^{12}$ cm^{-2} and still $k_F/q_0\approx0.8$ for our highest density. We, therefore, also ignore phase-space restriction.
[18] S. Das Sarma, Phys. Rev. B **27**, 2590 (1983).
[19] W. E. Carlos, J. A. Freitas Jr., M. A. Khan, D. T. Olson, and J. N. Kuznia, Phys. Rev. B **48**, 17878 (1993).
[20] M. W. Bayerl, M. S. Brandt, T. Graf, O. Ambacher, J. A. Majewski, M. Suitzmann, D. J. As, and K. Lischka, Phys. Rev. B **63**, 165204 (2001).
[21] C. Hermann and C. Weisbuch, Phys. Rev. B **15**, 823 (1977).
[22] T. A. Kennedy, E. R. Glaser, W. E. Carlos, P. P. Ruden, and S. Nakamura, MRS Internet J. Nitride Semicond. Res. **4S1**, G7.4 (1999).