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Transport-to-Quantum Lifetime Ratios in AlGaN/GaN Heterostructures

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Abstract: We have calculated ratios of the transport to quantum lifetimes τ/τ_q of the two dimensional electron gas in AlGaN/GaN heterostructures at low temperatures. In contrast to conventional interpretations, we show that large values of this ratio do not necessarily indicate that long-range scattering mechanisms such as Coulomb scattering are the dominant carrier scattering mechanisms and that large ratios (>20) can be obtained even when short range scattering mechanisms are dominant.

The performance of electronic devices based on AlGaN/GaN heterostructures is, to a large extent, determined by the transport properties of the two-dimensional electron gas (2 DEG) confined at the AlGaN/GaN interface. Although recent experimental and theoretical efforts have led to the identification of the major scattering mechanisms limiting the 2 DEG mobility, the relative importance of those scattering processes is still a hotly debated issue. One way to assess the relative importance of different scattering mechanisms is to measure the ratio of the transport to quantum relaxation times τ_t and τ_q [1-5]. The transport lifetime is typically calculated from Hall mobility measurements and the quantum lifetime can be determined from an analysis of the magnetic field dependence of Shubnikov-de Haas oscillations.

The difference between the two lifetimes lies in the averaging of scattering events over all angles. The quantum lifetime τ_q is a measure of the mean time a carrier remains in a particular state before being scattered to a different state. Thus, in calculations of the quantum lifetime, all scattering events are weighted equally. In contrast, the transport time τ_t is a measure of the amount of time a carrier remains moving in a particular direction. Thus, in calculating the transport lifetime, the inclusion of a factor of $1-\cos \theta$, where θ is the scattering angle, emphasizes the importance of large angle over small angle scattering events [6]. Consequently the lifetime ratio τ_t/τ_q is determined by the angular dependence of the matrix element for a given scattering process and it has been used to make inferences about the type of scattering mechanisms which limit the carrier mobility at low temperatures [1-5].

For example, for short range scattering potentials such as alloy disorder scattering, the matrix elements are mostly isotropic and the values of both the quantum and transport lifetimes are very similar, $\tau_t/\tau_q \approx 1$. For long range scattering potentials, such as Coulomb fields of background charges in the quantum well, this ratio is larger than 1. The largest values of the

τ/τ_q ratios are expected for scattering by remote Coulomb centers. In this case, the scattering matrix element has a strong angular dependence and is largest for small scattering angles. This leads to transport lifetimes which are much longer than quantum lifetimes since the inclusion of the factor of $(1-\cos(\theta))$ greatly reduces the average scattering rate when calculating the transport lifetime. Based on such an analysis it has been argued that an experimental observation of $\tau/\tau_q \sim 1$ can be interpreted as evidence that short-range potentials such as those generated by alloy disorder or interface roughness are the dominant mobility-limiting mechanisms. An experimental observation of $\tau/\tau_q \gg 1$ would indicate that long-range potentials such as the Coulomb fields generated by ionized impurities are the dominant mobility-limiting mechanisms.

It is important to note that in most cases, the transport and quantum lifetimes measured in experiments are determined by several different scattering processes and that the common interpretation of the lifetime ratio is valid only if both lifetimes are dominated by the same scattering process.

In this paper, we present theoretical calculations of the low-temperature transport and quantum lifetimes of the 2 DEG in AlGa_xN/GaN heterostructures. Our calculations show that in typical AlGa_xN/GaN heterostructures, the transport and quantum lifetimes are dominated by different scattering mechanisms, and thus that the experimentally determined values of τ/τ_q ratios cannot alone be used to identify the nature of the dominant scattering mechanism.

Low temperature quantum and transport lifetimes for 2 DEG electrons in nitride heterostructures were calculated incorporating all the standard scattering mechanisms, including acoustic phonons (both deformation potential and piezoelectric modes), alloy disorder, and Coulomb scattering due to both remote impurities in the AlGa_xN barrier and residual impurities in

the GaN quantum well. The inverse lifetimes for a particular mechanism are given by the following familiar expressions [6]:

$$\frac{1}{\tau_t} = \frac{m^*}{\pi \hbar^3 k_f^2} \int_0^{2k_f} \frac{q^2}{\sqrt{4k_f^2 - q^2}} \frac{U_q^2}{(1 + H(q))^2} dq \quad (1)$$

$$\frac{1}{\tau_q} = \frac{2m^*}{\pi \hbar^3} \int_0^{2k_f} \frac{1}{\sqrt{4k_f^2 - q^2}} \frac{U_q^2}{(1 + H(q))^2} dq \quad (2)$$

where U_q^2 is the scattering function, which depends on the particular mechanism, $H(q)$ is the standard Thomas-Fermi screening function [7], and k_F is the Fermi wavevector. These expressions were used to calculate the transport and quantum lifetimes [8]. The one exception was the calculation of the lifetimes due to scattering from residual charged centers in the GaN quantum well. In this case, the lowest order expression for the quantum lifetime is logarithmically divergent and the higher order multiple-scattering theory developed by Gold [9] was used.

Figure 1 shows calculated mobilities for a $\text{Al}_{0.15}\text{Ga}_{0.85}\text{N}/\text{GaN}$ heterostructure as a function of 2 DEG density. The range of 2 DEG densities shown corresponds to barrier thicknesses ranging from $\sim 50 \text{ \AA}$ to 500 \AA and were obtained through a self-consistent calculation assuming that the 2 DEG electrons originate from donor-like defects on the surface of the barrier [10,11]. The other parameters used in these calculations are listed in Table 1.

In addition to the total mobility, component mobilities for the three most important scattering mechanisms are shown. At low carrier densities, Coulomb scattering from charged unintentional impurities in the well and remote charges are the dominant scattering mechanisms. At high 2 DEG densities and higher electron energies, Coulomb scattering is much less effective and alloy disorder scattering, resulting from the penetration of the 2 DEG into the AlGa_N barrier, is the dominant scattering mechanism. Since the transport lifetime is directly proportional to the

Hall mobility $\tau_t = m^* \mu / e$, the vertical axes of figure 1 indicate the transport lifetimes corresponding to each of these mechanisms, in addition to the mobility. Results for heterostructures with other Al fractions are similar and show the same trend in which the scattering process responsible for limiting the transport time is Coulomb scattering at small carrier densities and alloy disorder scattering at high densities.

Figure 2 shows calculated quantum lifetimes for various scattering processes for the same heterostructure as in figure 1. In contrast to the transport lifetime, the quantum lifetime τ_q is dominated by scattering from remote charged impurities over the entire 2 DEG concentration range shown. Scattering by these impurities is dominant because of the large contribution of small angle scattering events to τ_q . In the case of the transport lifetime τ_t , the effectiveness of these scattering events is greatly reduced by the $(1 - \cos(\theta))$ factor. As is seen in figures 1 and 2, this difference is especially evident at larger 2 DEG densities where the τ_t / τ_q ratio for scattering by remote charged impurities can be larger than 100.

Figure 3 shows the lifetime ratio τ_t / τ_q for AlGaN/GaN heterostructures with three different Al fractions in the barrier. In all cases, the quantum lifetimes were only weakly dependent on the 2 DEG density and the transport lifetimes had maxima at the carrier densities at which Coulomb scattering and alloy disorder scattering were of approximately equal importance. Contrary to the usual interpretation of the lifetime ratio τ_t / τ_q , the largest values are obtained not when long-range scattering mechanisms are dominant, but when both short and long range scattering mechanisms contribute to the total scattering. Furthermore, at 2 DEG densities between $4 \times 10^{12} \text{ cm}^{-2}$ and $6 \times 10^{12} \text{ cm}^{-2}$ when the short-range alloy disorder potential is the dominant scattering mechanism, the value of τ_t / τ_q for the $\text{Al}_{0.15}\text{Ga}_{0.85}\text{N}/\text{GaN}$ heterostructure is still fairly large (> 20). In addition, one can see from figure 3 that at very low 2 DEG densities,

when the long range Coulomb potential is the dominant scattering mechanism, the value of τ/τ_q is close to one. This is because these low 2 DEG densities occur when the barrier is very thin and the carriers are located close to the scattering centers. In such a situation, large angle scattering events dominate both quantum and transport lifetimes and are nearly as common as small angle scatterings.

With a few exceptions, most of the τ/τ_q ratios that have been measured experimentally are between 1.5 and 9 [3,4,5] and are much lower than would be expected from calculations for equivalent heterostructures. However, the 2 DEG mobilities in these structures are also much lower than would be expected (much less than $10,000 \text{ cm}^2/\text{Vs}$ at 4 K). In this case, it is possible that a strong short-range scattering mechanism such as interface roughness scattering is the dominant factor limiting the carrier mobility. We calculated the transport and quantum scattering times, adding interface roughness scattering using the same formalism and parameters as described in reference 11. We found that the addition of this scattering mechanism leads to a significant lowering of both the low temperature mobility and the τ/τ_q ratio, especially at carrier densities above 10^{12} cm^{-2} . Thus in this case, small τ/τ_q ratios in low mobility samples might be indicative of the importance of interface roughness scattering in limiting the electron mobility. It should be noted that the heterostructure with the highest reported mobility of over $60,000 \text{ cm}^2/\text{Vs}$ [1] also has the highest lifetime ratio $\tau/\tau_q > 20$.

In conclusion, we have calculated the transport to quantum lifetime ratios in AlGaIn/GaN heterostructures. We find that, in contrast with traditional interpretations, large and small τ/τ_q ratios do not necessarily indicate which type of scattering mechanisms are dominant in a crystal. However, the unusually low (1.5 to 9) τ/τ_q ratios accompanied by very low low-temperature mobilities which have been reported in several studies may well indicate that a strong short-

range scattering mechanism, such as interface roughness scattering, is the dominant factor limiting the 2 DEG mobilities in those structures.

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Figure Captions

Figure 1. The density dependence of the total and three most important component mobilities in a $\text{Al}_{0.15}\text{Ga}_{0.85}\text{N}/\text{GaN}$ heterostructure. The component scattering mechanisms shown are Coulomb scattering from residual impurities in the GaN well, Coulomb scattering from remote donors in the AlGaN barrier, and alloy disorder scattering. The AlGaN barrier thickness ranges from $\sim 50\text{\AA}$ to 500\AA . Other parameters of this heterostructure are listed in Table I.

Figure 2. Combined and component quantum lifetimes in a $\text{Al}_{0.15}\text{Ga}_{0.85}\text{N}/\text{GaN}$ heterostructure. The component scattering mechanisms shown are alloy disorder scattering and Coulomb scattering from both residual impurities in the GaN well and remote donors in the AlGaN barrier.

Figure 3. Low-temperature (4K) values of the transport-to-quantum lifetime ratios for three different AlGaN/GaN heterostructures with different fractions of Al in the barrier.

Table I. Characteristics of the AlGaN/GaN heterostructures assumed for this calculation.

Growth temperature	800 °C
GaN deformation potential	9.5 eV
GaN elastic constants c_L	$35.5 \times 10^{12} \text{ N/m}^2$
c_T	$12 \times 10^{12} \text{ N/m}^2$
GaN piezoelectric constant h_{14}	$4.28 \times 10^9 \text{ V/m}$
AlN/GaN conduction band offset	2.1 eV
Residual n-type impurities in heterostructure	$2 \times 10^{16} \text{ cm}^{-3}$
Residual p-type impurities in GaN well	$1 \times 10^{16} \text{ cm}^{-3}$

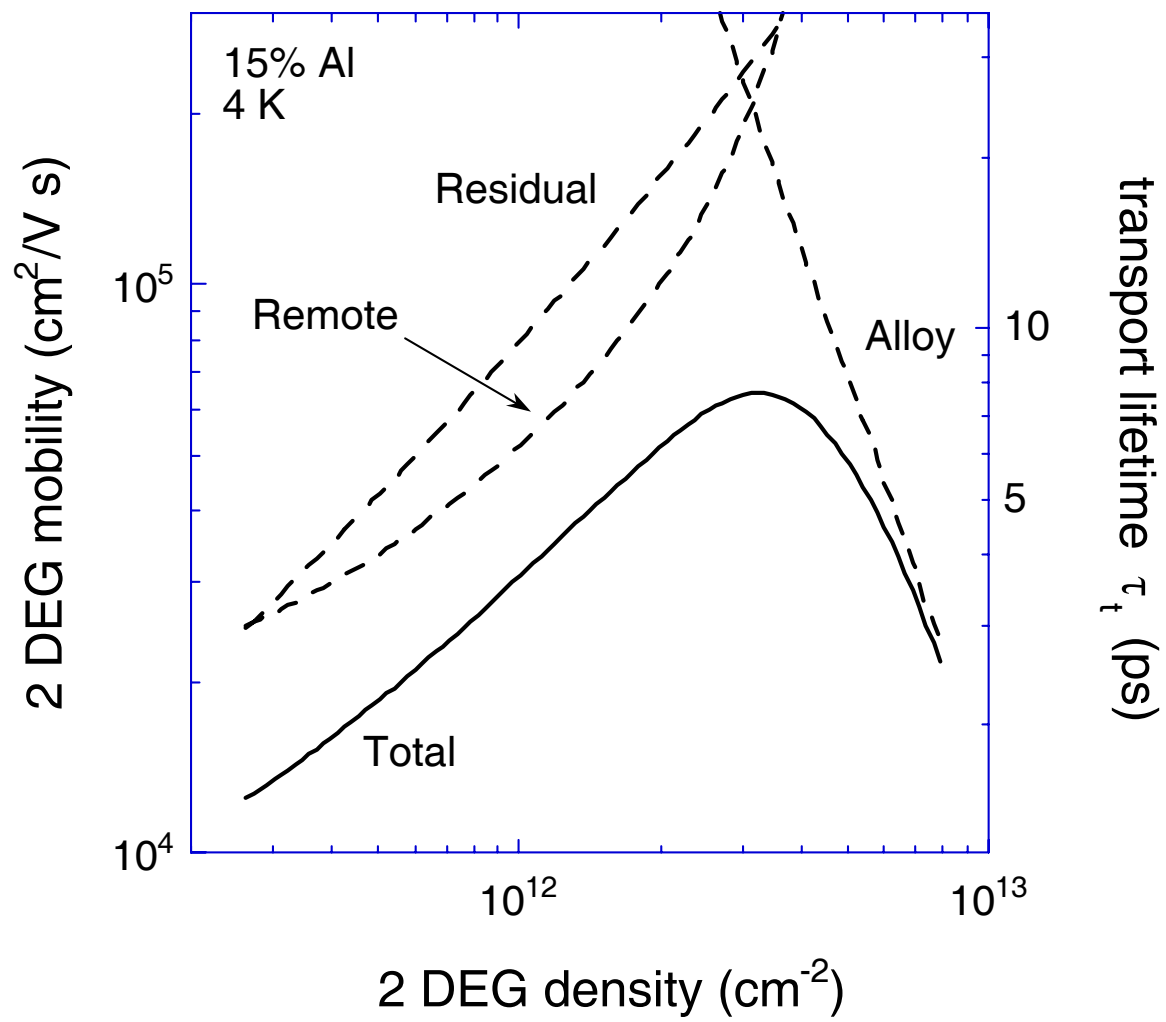


Figure 1

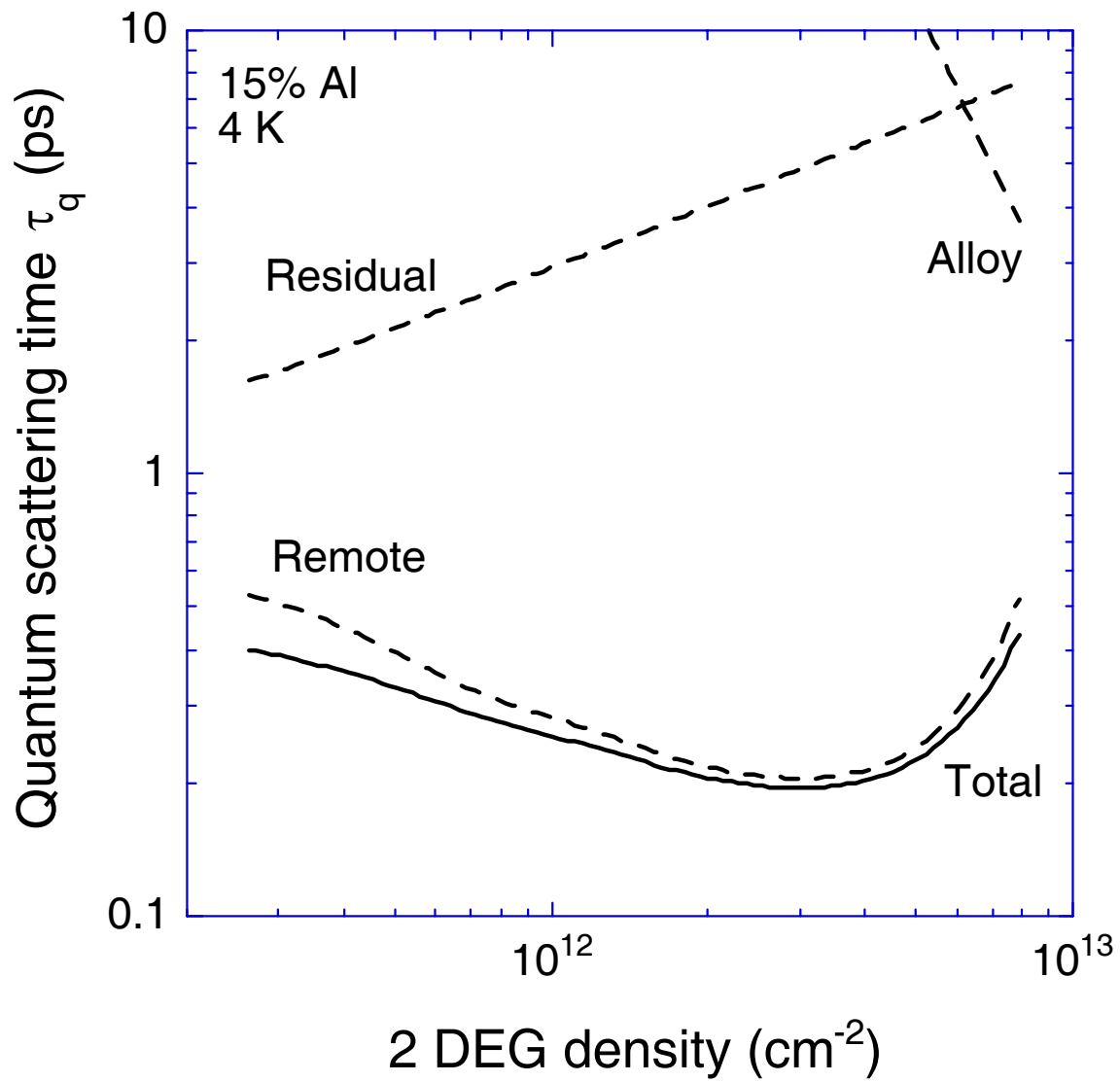


Figure 2

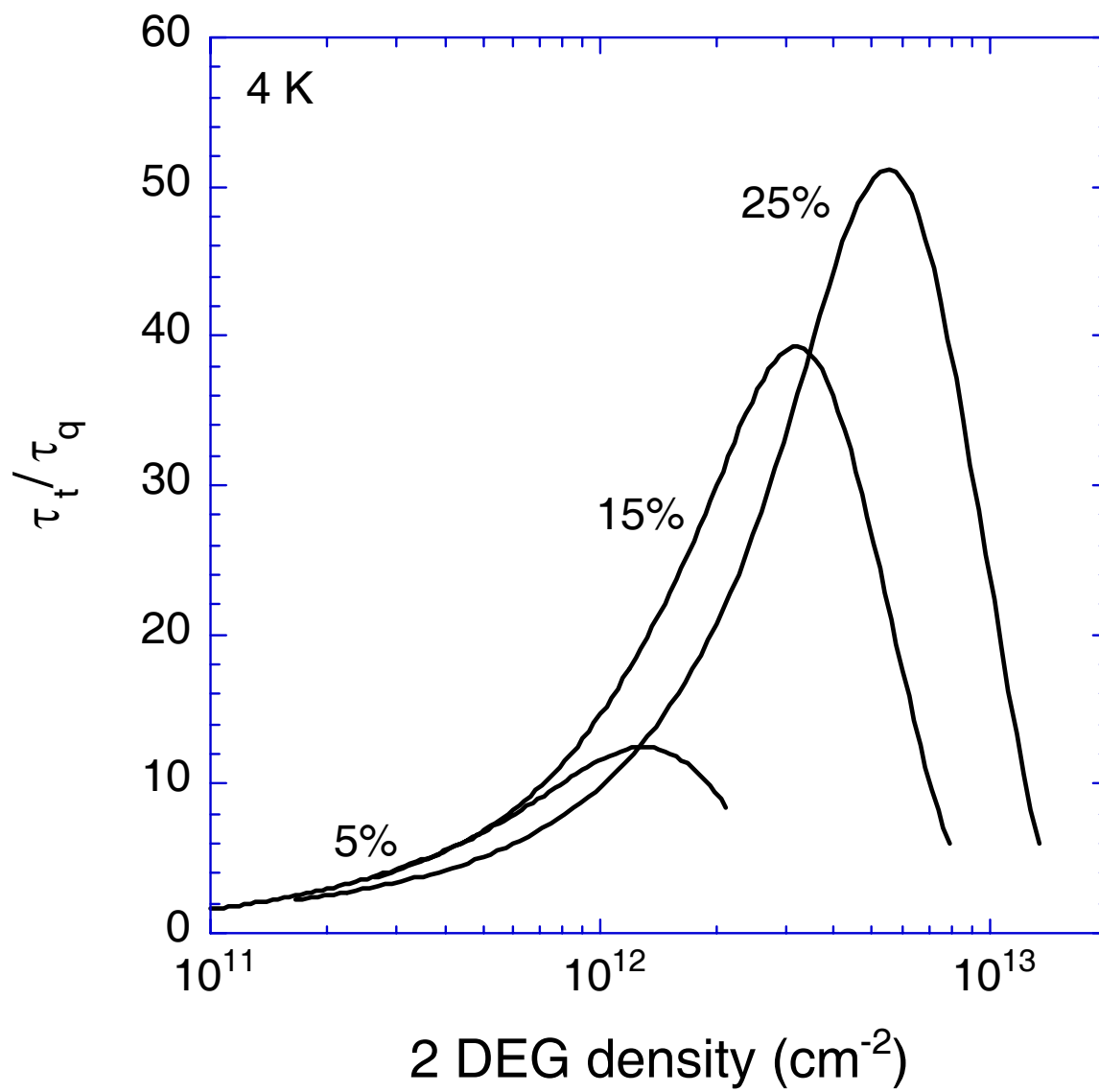


Figure 3