Scattering lifetimes due to interface roughness with large lateral correlation length in AlₓGa₁₋ₓN/GaN two-dimensional electron gas

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AlₓGa₁₋ₓN/GaN two-dimensional electron gas structures have been grown by molecular-beam epitaxy and exhibited surface roughness defined by the faceted surface morphology of the crystal grains or subgrains, with the grain size being the obvious lateral periodicity. The roughness amplitude varied in a wide range depending on the substrate type and growth conditions. The effect of interface roughness with lateral correlation length of the order of the grain sizes (0.1–1 μm) on the scattering lifetimes is calculated theoretically and compared with experimentally observed lifetime values. We conclude that scattering by long-range interface roughness has little impact on the transport lifetime, but competes with other scattering mechanisms to be the dominant source of small-angle scattering that limits the quantum scattering lifetime.

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I. INTRODUCTION

There has been increasing effort and incentives to understand the electrical transport mechanisms of the two-dimensional electron gas (2DEG) formed by AlₓGa₁₋ₓN/GaN heterostructures since these structures demonstrated extraordinary potential for high-power and microwave applications. The electrical properties of AlₓGa₁₋ₓN/GaN 2DEG’s grown by metal-organic chemical vapor deposition (MOCVD) and molecular-beam epitaxy (MBE) have been widely investigated by low-field as well as high-field transport measurements.¹–⁸ With recent advances in the growth techniques, low-temperature Hall mobilities of >10,000 cm²/V s and high-field Hall mobilities of up to 60,000 cm²/V s have been reported for AlₓGa₁₋ₓN/GaN 2DEG structures grown by both MBE and MOCVD.⁴⁻⁹ A number of theoretical works have also been published aiming to quantify the various scattering mechanisms in this system.¹⁴⁻¹⁷

One of the insufficiently understood behaviors of the AlₓGa₁₋ₓN/GaN 2DEG system is the large (> 6) and often unpredictably varied ratio between the measured transport scattering time τᵣ and the quantum scattering lifetime τᵣ₉. The transport scattering time is normally derived from the low-field mobility from the relation μᵣ = eτᵣ/m, whereas the quantum scattering time is determined from the Dingle plot of the amplitude of the Shubnikov–de Haas (SdH) quantum oscillations in the longitudinal magnetoresistance, which is a measure of the broadening of the Landau levels due to carrier scattering. Most studies conclude that small-angle scatterings are dominant in these AlₓGa₁₋ₓN/GaN structures. However, few studies have quantitatively identified the major source of small-angle scatterings in specific AlₓGa₁₋ₓN/GaN samples grown by any given technique (MOCVD or MBE).

AlₓGa₁₋ₓN/GaN 2DEG structures have been grown and studied in our laboratory for a number of years using the ammonia MBE growth technique. High mobilities of up to 14,500 cm²/V s have been observed, indicating good material quality. However, a perplexing phenomenon was observed that two samples having equal Hall mobilities could show very different quantum mobilities (or lifetimes). Studying of a series of samples revealed that decrease in quantum lifetime was often correlated with increasing surface roughness. Unlike the layers grown by MOCVD under optimized conditions, which typically show atomic-scale surface smoothness, the layers grown by ammonia MBE generally show a higher degree of surface roughness varying with substrate types and growth conditions. The defining roughness feature, as observed by atomic force microscopy (AFM), is the faceted surface morphology of the oriented hexagonal grains (or subgrains) with grain sizes typically larger than 0.3 μm for all the samples showing high Hall mobilities. This lateral scale of roughness defined by the grain structures is much larger than that of conventional atomic scale roughness, which is usually less than a few hundred angstroms. Note that these layers are single-crystalline films, with only a small twist existing between the oriented grains due to threading dislocations.¹⁸

In the present paper, the effect of scattering by this large lateral scale roughness has been studied on a series of samples covering a wide range of roughness amplitude. The transport and quantum lifetimes due to the roughness scattering were calculated theoretically using the measured roughness parameters (amplitude and lateral scale). Unlike some roughness scattering analysis where the roughness parameters were used as fitting parameters,¹⁹,²⁰ the present calculation of the scattering times using actual roughness values can be compared directly with experimental scattering times to determine if the roughness scattering is the limiting scattering mechanism.

II. EXPERIMENT

The AlₓGa₁₋ₓN/GaN 2DEG structures studied here were grown by the ammonia MBE method on sapphire and SiC
TABLE I. Surface roughness parameters and electrical transport properties determined for AlGaN/GaN 2DEG structures grown by ammonia MBE. \( \Delta \) and \( \Lambda \) are the rms amplitude and the lateral correlation length of the roughness, respectively. \( \mu_{\text{H}} \), \( \tau_r \), and \( \tau_q \) are the measured Hall mobility, transport scattering lifetime, and quantum scattering lifetime at 1.2 K, respectively. \( \tau_q^0 \) is the calculated roughness scattering lifetime at low temperature.

<table>
<thead>
<tr>
<th>Sample no.</th>
<th>Substrate</th>
<th>( \Delta ) (nm)</th>
<th>( \Lambda ) (nm)</th>
<th>( N_s ) ((10^{12} \text{ cm}^{-2}))</th>
<th>( \mu_{\text{H}} ) (cm²/V s)</th>
<th>( \tau_r ) (ps)</th>
<th>( \tau_q ) (ps)</th>
<th>( \tau_q^0 ) (ps)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0903</td>
<td>Sapphire</td>
<td>12.0</td>
<td>350</td>
<td>6.0</td>
<td>5.790</td>
<td>0.72</td>
<td>0.098</td>
<td>0.095</td>
</tr>
<tr>
<td>2310</td>
<td>Sapphire</td>
<td>63.5</td>
<td>1000</td>
<td>4.0</td>
<td>14.800</td>
<td>1.85</td>
<td>0.076</td>
<td>0.017</td>
</tr>
<tr>
<td>2410</td>
<td>SiC</td>
<td>8.5</td>
<td>550</td>
<td>4.0</td>
<td>11.300</td>
<td>1.41</td>
<td>0.158</td>
<td>0.485</td>
</tr>
<tr>
<td>2402</td>
<td>Sapphire</td>
<td>27.7</td>
<td>450</td>
<td>6.2</td>
<td>6.490</td>
<td>0.81</td>
<td>0.055</td>
<td>0.022</td>
</tr>
<tr>
<td>2502</td>
<td>Sapphire</td>
<td>18.1</td>
<td>450</td>
<td>4.5</td>
<td>8.130</td>
<td>1.02</td>
<td>0.058</td>
<td>0.045</td>
</tr>
<tr>
<td>2511</td>
<td>Sapphire</td>
<td>16.2</td>
<td>500</td>
<td>3.6</td>
<td>8.800</td>
<td>1.10</td>
<td>0.098</td>
<td>0.155</td>
</tr>
<tr>
<td>2801</td>
<td>MOCVD GaN</td>
<td>2.2</td>
<td>300</td>
<td>3.4</td>
<td>14.300</td>
<td>1.79</td>
<td>0.25</td>
<td>5.43</td>
</tr>
</tbody>
</table>

substrate and on MOCVD GaN/sapphire template substrates. The substrates appeared to have significant impact on the surface roughness. The highest degree of surface roughness was found in samples grown on sapphire substrates. The layers grown on the SiC substrates showed improved smoothness. The best smoothness was achieved on the layers grown on MOCVD GaN templates. Reduced lattice mismatch to the substrate clearly favored smoother growth. The fluctuation in growth conditions such as the growth temperature caused the variation of roughness among samples grown on the same kind of substrates.

For all samples except those grown on MOCVD templates, the growth was as follows. A 20-nm-thick AlN layer deposited in situ by magnetron sputter epitaxy was used as the buffer layer. The complete structure contains a 2-\( \mu \)m-thick undoped GaN channel layer and 20 nm of Al\(_{2}\)Ga\(_{1-x}\)N barrier layer. The Al concentration is roughly in the range 5–10%, resulting in 2DEG sheet densities from 3.4×10\(^{12}\) to 6.2×10\(^{12}\) cm\(^{-2}\) due to spontaneous and piezoelectric polarization effects. The growth was performed at 890 °CURL4521/5262 on 50-sccm (standard cubic centimeter) ammonia flow rate. More details on the growth technique and procedures have been published elsewhere.\(^{23,24}\)

For the growth on the MOCVD GaN template layer, no buffer layer was used, and a lower growth temperature of 800°C was used in order to prevent thermal decomposition of the GaN template layer. The MOCVD GaN layer was nominally undoped. The structure grown on the MOCVD GaN template contains 0.2 \( \mu \)m of undoped GaN channel layer and 20 nm of Al\(_{2}\)Ga\(_{1-x}\)N barrier layer.

The samples were cut to 5×5-mm squares for magnetoresistance measurements in the Van der Pauw geometry at low temperatures. Indium contacts were soldered on the four corners, and Ohmic linearity was verified. The transverse \( (R_{\perp}) \) and longitudinal \( (R_{\parallel}) \) resistance was measured at 1.2 K in magnetic fields up to 8 T.

The surface morphology of the samples was imaged using an atomic force microscope operating in the tapping mode. The root-mean-square (rms) values of the roughness amplitude (\( \Delta \)) and the average grain size or lateral scale of roughness (\( \Lambda \)) were obtained from 5×5-\( \mu \)m scans. Since the Al\(_{2}\)Ga\(_{1-x}\)N barrier was only 20 nm thick in all the samples, the surface roughness was found to reflect similar roughness at the Al\(_{2}\)Ga\(_{1-x}\)N/GaN interface. The identity of the samples included as well as the experimentally determined surface roughness parameters and electrical parameters is given in Table I.

### III. INTERFACE ROUGHNESS SCATTERING TIMES

For a two-dimensional electron gas occupying a single parabolic subband at low temperature, to the lowest order of the scattering potential, the transport lifetime and quantum lifetime due to interface roughness scattering are given by the well-known expressions\(^ {25,24}\)

\[
\frac{1}{\tau_i^{0}} = \frac{1}{2 \pi \hbar e_F} \int_{0}^{2k_F} \frac{q^2}{(4k_F^2 - q^2)^{1/2}} \frac{U_q^2}{e_q^2} dq = \frac{m}{\pi \hbar^2} \int_{0}^{\pi} dq \frac{U_q^2}{e_q^2} \theta(q),
\]

\[
\frac{1}{\tau_q^{0}} = \frac{1}{2 \pi \hbar e_F} \int_{0}^{2k_F} \frac{2k_F^2}{(4k_F^2 - q^2)^{1/2}} \frac{U_q^2}{e_q^2} dq = \frac{m}{\pi \hbar^2} \int_{0}^{\pi} dq \frac{U_q^2}{e_q^2} \theta(q),
\]

where \( q \) is the Thomas-Fermi screening wave number (parameter) given by \( q = m e^2 /2 \pi \epsilon_0 \gamma_s \hbar^2 \), \( m \), \( e_L \), and \( \epsilon_0 \) are the electron effective mass, the static dielectric constant of the semiconductor, and the vacuum dielectric constant, respectively. \( \theta(x) \) is a usual step function of \( x \). \( F(q) \) is a form factor given by\(^ {19,25}\)
Therefore, with $D_2 > 1$ since $1 - \cos \theta$ for the transport time, but not for the quantum time. If the scattering events are predominantly small-angle scatterings, the $\tau_\text{q}/\tau_\text{q}$ ratio will be larger than unity since $1 - \cos \theta$ diminishes at small $\theta$. It is easy to see from the equations above that the amplitude of the roughness $\Delta$ factors out as a simple scaling parameter in the calculation of the total scattering rate and has no effect on the angular dependence. On the other hand, the lateral correlation scale of the roughness $\Lambda$ is a determining factor to the angular dependence of the scattering. For large $\Lambda$, the exponential term in the scattering potential in Eq. (8) will fall off rapidly with increasing $q$, making the scattering important only at small angles. Thus, the value of $\Lambda$ has effect on the form and behavior of $\omega_q$ (or $\theta$), as will be further elucidated in the discussion of the measurement and calculation results in the following section.

IV. RESULTS AND DISCUSSION

Among the samples listed in Table I, samples 2310 and 2801 exhibited almost the same highest Hall mobility observed in this group of samples of about 14 000 cm$^2$/V s (at 1.2 K) and similar 2DEG sheet densities. To our initial surprise, while sample 2801 showed the strongest SdH quantum oscillations, sample 2310 showed very weak, hardly noticeable oscillations. Figure 1 shows the longitudinal magnetoresistance ($R_{xx}$) measured at 1.2 K for these two samples. It is noteworthy that the SdH oscillations start below 2 T in sample 2801. In sample 2310 in contrast, the oscillations can only be noticed at high fields after the signal is subtracted from the nonoscillatory background and enlarged in scale, as shown by the inset graph in Fig. 1(b). The amplitude of the Shubnikov–de Haas oscillations is given by

$$\Delta R = 4R_0\chi(T)\exp(-\pi/\omega_c\tau_\text{q}),$$

FIG. 1. Magnetoresistance measured at 1.2 K for (a) sample 2801 and (b) sample 2310. The inset graph in part (b) is the scale-up of the oscillation part of the magnetoresistance of sample 2310.
where $R_0$ is the zero-field longitudinal resistance, $\omega_c$ the cyclotron frequency, and $X(T)$ a temperature damping factor given by

$$X(T) = \frac{(2\pi^2 kT/\hbar \omega_c)/\sinh(2\pi^2 kT/\hbar \omega_c)}{\sinh(2\pi^2 kT/\hbar \omega_c)}.$$  (10)

Equation (9) shows that the SdH oscillation strength is sensitively (exponentially) dependent on the quantum lifetime. The quantum lifetime is usually derived from the so-called Dingle plot. If $\Delta R/4R_0 X(T)$ is plotted in logarithm against $1/B$, the slope gives $1/\tau_q$ with an intercept of 1 at $1/B = 0$.

Figure 2 shows the Dingle plots for samples 2310 and 2801. The slopes of the curves give $\tau_q = 0.076$ ps and $\tau_q = 0.25$ ps for samples 2310 and 2801, respectively. The fact that the intercept at $B = 0$ is correct indicates that only one subband is occupied, as has been assumed. The $\tau_q$ values for the other samples were similarly determined and given in Table I.

The results in Figs. 1 and 2 reveal that sample 2310 has a significantly smaller quantum lifetime than sample 2801, though both samples show almost equal transport lifetimes. As pointed out in the preceding section, small-angle scattering has little effect on the transport lifetime, but does impact the quantum lifetime. In this case, the interface roughness appears to be a quite possible source of the small-angle scatterings because the two samples are on the opposite ends of the roughness range observed. Sample 2310 was grown on a sapphire wafer and shows extremely high rms roughness amplitude of 63.5 nm. In contrast, sample 2801 was grown on a MOCVD GaN template and shows a rms roughness amplitude of only 2.2 nm. The huge contrast of surface roughness of the two samples is illustrated by the AFM images in Fig. 3.

It is quite surprising that sample 2310, with such high roughness amplitude, can still show the highest Hall mobility in this group of samples. Apparently, the roughness scattering is not the limiting factor for the transport mobility (or lifetime) in this case. Though the amplitude of the roughness feature is huge, it is defined by the grain structures, whose lateral scale ($\Lambda$) corresponding with the grain sizes is on the order of micrometers in all the high-mobility samples studied here (see $\Lambda$ values in Table I). As we already pointed out, at large $\Lambda$, the interface roughness scattering is important only at small angles and affects only the quantum lifetime. Thus, when this scattering mechanism becomes more important in the Al$_x$Ga$_{1-x}$N/GaN 2DEG structures, we should expect to see an increase in the $\tau_t/\tau_q$ ratio.

In Fig. 4, the experimentally measured values of the $\tau_t/\tau_q$...
ratio from the samples in Table I are plotted against the roughness amplitude ($\Delta$) values. We can see a clear trend of correlation. At small $\Delta$, the ratio is around 7. Similar ratios were reported in the literature for MOCVD-grown Al$_x$Ga$_{1-x}$N/GaN structures.\cite{1,6} The MOCVD-grown structures typically show atomic-level smoothness. At the largest $\Delta$ value, the ratio climbed up to 25, indicating an increased component of small-angle scatterings. Equation (8) shows that the interface roughness scattering potential scales with square of the roughness amplitude ($D^2$). Thus, the trend shown in Fig. 4 strongly suggests that the scattering by interface roughness with a large lateral correlation length could well be a major source of small-angle scatterings.

The dependence of interface roughness scattering $\tau_i$ and $\tau_q$ on major sample parameters such as $\Delta$, $\Lambda$, and $N_s$ have been calculated from Eqs. (1)–(8). Figure 5 presents the calculated values of $\tau_i$ and $\tau_q$ as a function of the lateral length $\Lambda$ for given values of $\Delta$ (=10 nm) and $N_s$ (=6 x 10$^{12}$ cm$^{-2}$). At very small $\Lambda$ ($k_F\Lambda \ll 1$), $\tau_i/\tau_q = \frac{1}{2}$ is obtained in the calculation. At large $\Lambda$ ($k_F\Lambda \gg 1$), $\tau_i$ is shown to be proportional to $\Lambda^3$, whereas $\tau_q$ is proportional to $\Lambda$. Thus $\tau_i/\tau_q$ is proportional to $\Lambda^2$. These calculation results agree very well with the analytical results by Gold.\cite{25} The results attest to the fact that the lateral correlation length determines the scattering range. A $\tau_i/\tau_q$ ratio of about $\frac{1}{2}$ when $\Lambda \ll 1/k_F$ indicates that scattering by roughness of this short lateral scale is basically short-range, large-angle scattering. At $\Lambda \gg 1/k_F$, however, the $\tau_i/\tau_q$ ratio can span several orders of magnitude as shown in Fig. 5, indicating the scattering by roughness of large lateral scale is extremely long-range, small-angle scattering.

For the samples studied, the $\Lambda$ values are between 100 and 1000 nm, as determined from the average grain sizes observed. In this range of $\Lambda$, we see the calculated transport time $\tau_i$ due to roughness scattering is orders of magnitude higher than all the measured $\tau_q$ values. This is not surprising since the roughness scattering is of long-range and small-angle character. $\tau_i$ in this case should be limited by other short-range scatterings such as scattering by threading dislocations and ionized impurities in the channel. A recent experimental study of the electron transport mobility in MOCVD-grown GaN/Al$_x$Ga$_{1-x}$N/GaN structures has also found that the transport mobility does not show dependence on the surface roughness, rather, that it shows correlation with the columnar domain size (or grain size).\cite{29} Higher density of threading dislocations is generally associated with smaller grain size.

However, the calculated $\tau_q$ values fall into the same range as the measured $\tau_q$ values. The measured $\tau_q$ of sample 0903 is shown on the graph (the square) for comparison with the calculation. This sample can be directly shown on this graph because its parameters ($\Delta$ and $N_s$) are very close to those used for the calculation. We can see that the experimental point falls nicely on the theoretical curve. This result strongly suggests that the interface roughness scattering could be the dominant source of small-angle scattering in this sample. The $\tau_i/\tau_q$ ratio calculated from roughness scattering would be much higher than any measured values, because the actual $\tau_i$ is limited by other large-angle scattering mechanisms.

Though the theoretical curves in Fig. 5 are presented only for one set of $\Delta$ and $N_s$ values, they can also be easily adapted for other $\Delta$ values. The scattering lifetimes simply scale with $\Delta^2$. The form of the curves in the graph is independent of $\Delta$. However, the value of $N_s$ does influence the form as well as the magnitude of the curves.

Figure 6 shows a comparison of the calculated roughness scattering $\tau_q$ values with the measured values for all the samples studied, presented against the respective roughness amplitude of each sample. The actual measured $\Delta$, $\Lambda$, and $N_s$ values of each sample were used in calculating its $\tau_q$. We see that for samples with a roughness amplitude greater than 10 nm, the measured $\tau_q$ values are quite close to the roughness scattering times, indicating roughness scattering could be the major source of small-angle scattering in these samples. However, for samples showing small roughness amplitude (less than 10 nm), the measured $\tau_q$ does increase with decreasing roughness, but falls markedly below the calculated roughness scattering quantum time. This means when the interface roughness is reduced to a certain level, the
roughness scattering strength is greatly reduced so that it is no longer the limiting mechanism for small-angle scattering. Other types of small-angle scattering such as scattering by remote ionized centers may set in as the limiting mechanism.

The fact that $\tau_r/\tau_p$ ratios in the range of 5–8 are also commonly observed in high-quality MOCVD-grown Al$_x$Ga$_{1-x}$N/GaN 2DEG (Refs. 1 and 6) typically having atomically smooth interfaces also suggests that the usual type of small-angle scattering by remote ionized centers is still important in these structures. Theoretical treatment of the remote donor scattering in Al$_x$Ga$_{1-x}$N/GaN, however, is less obvious than in the Al$_x$Ga$_{1-x}$As/GaAs system. The 2DEG in the Al$_x$Ga$_{1-x}$N/GaN structures is induced by spontaneous and piezoelectric polarization effects. There is still controversy as to the nature and location of the sources of these charges.

The long-range interface roughness scattering analyzed in this work is in addition to the usual sources of small-angle scattering, and will become a dominant component only when the amplitude of the roughness is high enough. MBE-grown Al$_x$Ga$_{1-x}$N/GaN structures are typically much rougher than the MOCVD-grown counterparts. The roughness of the MBE-grown layers arises from the usual three-dimensional growth mode causing the crystal grains to form sloping facets on the top surface. The amplitude and lateral length of the roughness are thus easily recognizable from the height and lateral size of such grain morphologies. When studying transport properties of MBE samples with such morphologies, the interface roughness scattering phenomena as discussed in this work could be important to take into account.

Though MOCVD-grown layers are usually extremely smooth (rms roughness of about 0.1–0.2 nm), sometimes the smoothness holds only in a very small lateral scale. Wavy or patchy surface morphologies are sometimes observed due to strain or inhomogeneous growth conditions. Depending on the amplitude and wavelength of such long-range surface roughness, the small-angle scattering due to this kind of roughness may become important even in MOCVD-grown samples. There has been a report that SdH oscillations were totally washed out with no clear reason in a MOCVD-grown Al$_x$Ga$_{1-x}$N/GaN 2DEG with quite high Hall mobility. The interface roughness scattering could be a reason, though the surface roughness conditions were not described in the paper.

Finally, the accuracy of the calculations is certainly limited by the simple assumption of Gaussian-correlated roughness and the single-particle scattering approximation. Also only the large lateral length component of the roughness is considered since it is the most dominant roughness feature observed. Implications of shorter scale roughness components on transport and quantum scatter times were not included. To identify the shorter scale components would require more deliberate analysis of the AFM data. Nevertheless, the calculation results agree quite convincingly with the measurement data.

V. CONCLUSIONS

The scattering by interface roughness with the lateral correlation length of the order of the grain size (0.1–1 μm) in Al$_x$Ga$_{1-x}$N/GaN 2DEG structures was found to correlate with strong damping of the Shubnikov–de Haas quantum oscillations, but have little impact on the Hall mobility. Theoretical calculations have been performed and showed that scattering by interface roughness of such long lateral length is strong only at small angles. The transport lifetime calculated from the roughness scattering is much higher than the observed values, indicating that other short-range scattering mechanisms are limiting the transport lifetime in these structures. However, the quantum lifetime calculated from the roughness scattering agrees with the observed values for samples showing rms roughness amplitude greater than 10 nm. For samples with smaller roughness, the observed quantum lifetime increases with decreasing roughness amplitude, but falls significantly below the theoretical value for roughness scattering. This means other sources of small-angle scattering such as remote donors are competing with the interface roughness in being the limiting factor of the quantum lifetime. The roughness scattering analysis was performed on MBE-grown samples where the surface roughness was defined by the faceted surface of its grained structure. A similar analysis may also be applicable for MOCVD-grown samples with other types of long-range roughness features.

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SCATTERING LIFETIMES DUE TO INTERFACE . . .
