Electron mobility in graded AlGaN alloys

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Polarization gradients in graded AlGaN alloys induce bulk electron distributions without the use of impurity doping. Since the alloy composition is not constant in these structures, the electron scattering rates vary across the structure. Capacitance and conductivity measurements on field effect transistors were used to find mobility as a function of depth. The effective electron mobility at different depths calculated from theory closely matched the measured mobility. Local bulk mobility values for different AlGaN compositions were found, and the electron mobility in AlGaN as a function of alloy composition was deduced. These were found to match with theoretical calculations. © 2006 American Institute of Physics. [DOI: 10.1063/1.2165190]

Gallium nitride and related alloys have higher spontaneous and piezoelectric polarization than other III–V semiconductors. In AlGaN/GaN heterostructures, the piezoelectric polarization in the strained AlGaN and the discontinuity in the spontaneous polarization at the heterointerface leads to a fixed sheet charge at the heterointerface. This is used in AlGaN/GaN high electron mobility transistors where a two-dimensional electron gas is formed to screen the net positive fixed sheet charge at the heterointerface. This is achieved by grading the Al composition in the AlGaN alloy, thus creating a polarization gradient in the graded region. The polarization-induced carrier density, \( \rho_p \), is given by the equation

\[
\rho_p = \nabla \cdot \mathbf{P},
\]

where \( \mathbf{P} \) is the total polarization in the material. The polarization \( \mathbf{P} \) here is the sum of the spontaneous and piezoelectric polarization in the AlGaN alloy and can be approximated by using Vegard’s law for the elastic constants. Transistors based on graded AlGaN alloys have been predicted to be technologically important for microwave applications.\(^7,8\)

In this work, we compare measurements and theoretical calculations of mobility for polarization-induced three-dimensional electron gases in graded AlGaN alloys. The electrical and physical properties vary in the growth direction in graded AlGaN alloys because of the continuously changing Al composition. Electron scattering rates are therefore different in different parts of the channel depending upon the local alloy composition, and these must be taken into account while calculating or analyzing electron mobility in graded alloys.

The effective electron scattering rate (proportional to \( 1/\mu_{\text{eff}} \)) is given by the first moment of the electron density \( [n(z)] \) with respect to the local scattering rate [proportional to \( 1/\mu(z) \)].

\[
\frac{1}{\mu_{\text{eff}}(z)} = \int \frac{n(z)}{\mu(z)} dz, \tag{2}
\]

Here, \( \mu(z) \) is the mobility for an electron gas of density \( n(z) \) in a bulk AlGaN slab with the composition \( x_{\text{Al}}(z) \). Calculations for graded AlGaN layers\(^4\) have shown that the dominant scattering mechanisms limiting effective electron mobility at room temperature are alloy scattering and optical phonon scattering. In bulk GaN, Chin et al.\(^9\) have shown that optical phonon scattering is the dominant mechanism at room temperatures. In the present work, we therefore take into account only alloy scattering and optical phonon scattering to calculate the bulk mobility in AlGaN alloys

\[
\frac{1}{\mu(z)} = \frac{1}{\mu_{\text{op}}(z)} + \frac{1}{\mu_{\text{alloy}}(z)}. \tag{3}
\]

![FIG. 1. A three-dimensional electron gas induced in graded AlGaN. The coordinate “z” used in the equations is shown for reference.](image)

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The alloy scattering-limited mobility in an AlGaN alloy with Al composition $x_{Al}(z)$ is given by the expression:

$$\frac{1}{\mu_{alloy}(z)} = \frac{2q\hbar kT \ln[1 + \exp(E_f(z)/kT)]}{3\pi n_e(z) V_0(z)^2 \Omega_0(z) n(z)x_{Al}(z)[1 - x_{Al}(z)]}$$

(4)

Here, $V_0$ is the alloy scattering potential for (Al,Ga)N alloys which has been found to be 1.8 eV from magnetotransport measurements on similar structures.\(^5\) The unit cell volume $\Omega_0(z)$ was calculated for different alloy compositions by linearly interpolating lattice and elastic constants between GaN and AlN, and $m_e$ is the effective mass of electrons (Table I). $n(z)$ is the electron density measured by capacitance-voltage (C-V) profiling. $E_f(z)$, the position of the Fermi level with respect to the conduction band is found using the Joyce-Dixon approximation\(^6\):

$$E_{JD} = kT \left[ \ln \left( \frac{n(z)}{N_c(z)} \right) + A1 \left( \frac{n(z)}{N_c(z)} \right) + A2 \left( \frac{n(z)}{N_c(z)} \right)^2 \right],$$

(5)

where the constants $A1$ and $A2$ are $1/\sqrt{8}$ and $-4.950 09 \times 10^{-3}$, respectively, and $N_c(z)$ is the conduction band density of states of the AlGaN alloy in a region with composition $x_{Al}(z)$. This was calculated by interpolating between the values (Table I) for AlN and GaN.

The optical phonon scattering rate is given by

$$\mu_{op} = \frac{4 \pi e_0^2 (z) \hbar}{q m_e(z) \epsilon_0(z) N_{BE}(z)},$$

(6)

where $e_0$ is the permittivity of vacuum, $\epsilon^* = 1/\epsilon_0(z)$ $-1/\epsilon_0(z)$, $m_e(z)$ is the electron effective mass, $q_0(z)$ is the optical phonon energy, and $N_{BE}(z)$ is the Bose-Einstein phonon number in an AlGaN alloy with composition $x_{Al}(z)$. The constants for the AlGaN alloy were calculated by linear interpolation between the respective values for AlN and GaN (Table I).

The structure used in these experiments was grown on a sapphire substrate by metalorganic chemical vapor deposition. It consists of an insulating GaN buffer,\(^4\) an AlGaN region linearly graded from 0% to 30% over 100 nm and a 5 nm GaN layer. Transistors and capacitors were fabricated on this epilayer using standard processing techniques. Ti/Al/Ni/Au contacts were deposited and annealed at 870 °C for 30 s, mesa isolation was achieved using Cl$_2$-based reactive ion etching, and a Ni/Au metal layer was deposited for gate contacts.

Electron mobility in these structures were measured using a combination of transistor $I$-$V$ measurements and $C$-$V$ profiling. First, the charge as a function of depletion distance, $n(z)$, was calculated from $C$-$V$ measurements, as shown in Fig. 2. Since this structure was not doped, the total integrated charge for depletion depth can be related to the composition at that depth using Eq. (1). The calculated composition versus depth profiles (Fig. 2, inset) are used in the theoretical calculations of mobility.

A small current (100 μA) was forced between the source and drain of the transistor for different gate voltages and the voltage drop between source and drain ($V_{DS}$) was recorded. The voltage drop in the channel region under the gate is given by

$$V_{CH} = V_{DS} - I_{DS}(R_S + R_D).$$

(7)

The source and drain access resistances, $R_S$ and $R_D$, were estimated using the sheet resistance and contact resistance estimated from transfer length method measurements. Since a very small current was applied, we assume that the lateral electric field and charge distribution under the gate is uniform. With this assumption, the mobility at any gate voltage $V_G$ is given by the equation

$$\mu_v(V_G) = \frac{I_{DS}}{q n(z) V_{DS} V_G / L_g},$$

(8)

where $n(z)$ is the total sheet charge at a gate bias $V_G$ (calculated from $C$-$V$ measurements) and $L_g$ is the gate length (0.7 μm). Since the depletion depth at each gate voltage is known from $C$-$V$ profiling, the mobility as a function of depletion depth can be calculated. Measured and calculated electron mobilities for different depletion depths, shown in Fig. 3, show good agreement. As expected the channel has the highest mobility close to depletion where most of the charge is in low composition AlGaN and there is less alloy scattering.

**TABLE I.** Material constants for GaN and AlN.

<table>
<thead>
<tr>
<th>Constant</th>
<th>GaN</th>
<th>AlN</th>
<th>Units</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Effective mass</td>
<td>$m_e$</td>
<td>0.228</td>
<td>0.35</td>
<td>8 and 9</td>
</tr>
<tr>
<td>Lattice constant</td>
<td>$a$</td>
<td>3.19</td>
<td>3.11</td>
<td>10</td>
</tr>
<tr>
<td>Elastic constant</td>
<td>$c$</td>
<td>5.18</td>
<td>4.98</td>
<td>10</td>
</tr>
<tr>
<td>Elastic constant</td>
<td>$c_{13}$</td>
<td>103</td>
<td>108</td>
<td>GPa 11</td>
</tr>
<tr>
<td>Elastic constant</td>
<td>$c_{33}$</td>
<td>398</td>
<td>373</td>
<td>GPa 11</td>
</tr>
<tr>
<td>Optical phonon energy</td>
<td>$\hbar\omega_{op}$</td>
<td>91.2</td>
<td>99.2</td>
<td>meV 12</td>
</tr>
<tr>
<td>Low frequency dielectric constant</td>
<td>$\epsilon_0$</td>
<td>9.7</td>
<td>8.5</td>
<td>13</td>
</tr>
<tr>
<td>High frequency dielectric constant</td>
<td>$\epsilon_s$</td>
<td>5.3</td>
<td>4.6</td>
<td>13</td>
</tr>
</tbody>
</table>

**FIG. 2.** Carrier concentration vs depth. The inset shows the calculated Al composition at each depth.
These measurements also confirm measurements of the alloy scattering potential by Jena et al. The information from these measurements can also be used to calculate the mobility as a function of Al composition. Equation (2) can be rearranged and discretized to give

$$\frac{n_k}{\mu_k} = \frac{n_{S,K-1}}{\mu_{eff,K}} - \frac{n_{S,K}}{\mu_{eff,K-1}}$$

(9)

where $n_k$ is the integrated sheet carrier densities in the undepleted region up to the $K$th region, $\mu_{eff,K}$ is the effective mobility of that sheet, and $n_k$ is the sheet charge in the $K$th discrete region. Therefore, since the effective mobility at different depletion depths and the associated sheet charge are known, the bulk mobility for the Al composition at each of these points can be calculated.

The mobility values calculated using this method are compared with the theoretical bulk mobility [from Eq. (3)] in Fig. 4. The alloy and optical phonon-limited mobilities from theory are also shown. At lower Al compositions, the mobility is limited mainly by optical phonon scattering whereas at Al compositions greater than around 0.14 the mobility is mainly alloy-scattering limited. At very low GaN compositions (below 0.5%) the measured mobility shown in the plot is higher than the calculated mobility. The measurement in this regime may be affected by variations in the epitaxial layers between the C-V patterns and the transistors. Further, since the sheet density is low and the lateral electric fields are high, the simple relations applied to calculate the mobility are no longer valid. At higher Al compositions, however, there is a good match between the measured and theoretical values of mobility.

In conclusion, the effective mobility as a function of depletion depth in graded AlGaN alloys was calculated taking into account alloy and optical phonon scattering. Experimental mobilities were estimated using transistor $I$-$V$ and capacitance-voltage measurements. A good match was found between the experimental and theoretical values. The bulk AlGaN mobilities as a function of alloy composition were also estimated from these measurements and were found to agree well with the theoretically predicted values. The mobility characterization may be used in the analysis and design of transistors based on these graded AlGaN layers.

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