Predicted Maximum Mobility in Bulk GaN

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The last decade has seen a surge in research and development on GaN-related materials and devices. The driving force has been the potential for blue/UV light-emitting diodes (LEDs) and laser diodes, and also high-frequency transistors operating at high powers and temperatures. In fact, blue LEDs have already been commercialized, and blue lasers will soon be employed in consumer products. However, these successes are a mystery to many researchers, because even the best GaN materials have high concentrations of donors, acceptors, point defects, and dislocations, compared with those of, say, Si and GaAs. Moreover, it is generally acknowledged that development of commercial electronic devices, and further improvements in photonic devices, will require better materials. Recently, a marked improvement in electron mobility, the most commonly used figure of merit, has been realized by two types of GaN growth: (1) hydride vapor-phase epitaxy (HVPE) on Al$_2$O$_3$, with subsequent separation of the GaN from the Al$_2$O$_3$, and (2) molecular-beam epitaxy on templates consisting of metal–organic chemical-vapor deposition on Al$_2$O$_3$. Each of these techniques has produced a sample with a 300 K mobility of close to 1200 cm$^2$/V s, a world’s record for bulk (three-dimensional) conduction in GaN. (Of course, two-dimensional mobilities in AlGaN/GaN heterostructures can be significantly higher because of confinement and screening effects.) In this article, we fit the temperature-dependent mobility $\mu$ and carrier concentration $n$ of the highest-mobility bulk GaN sample available to get accurate values of donor concentration $N_D$, acceptor concentration $N_A$, donor activation energy $E_D$, acoustic-mode deformation potential $E_1$, and piezoelectric coefficient $P$ (or piezoelectric constant $h_{pz}$). Other, better-known parameters important for scattering, such as the effective mass, are taken from the literature. Fortunately, the fitted values of $E_1$ and $h_{pz}$ are quite representative of those available in the literature, giving credence to our model. We then can calculate mobility curves for the smallest estimated realistic values of $N_D$ and $N_A$, and thus find the maximum mobility in bulk GaN at a given temperature.

The GaN sample discussed here was grown in the (0001) orientation (Ga face up) on Al$_2$O$_3$ by the HVPE technique at the Samsung Advanced Institute of Technology. Separation of the GaN and Al$_2$O$_3$ was effected by laser irradiation on the N face, through the Al$_2$O$_3$ substrate. This particular sample, as well as several others prepared in the same way, have been extensively characterized by optical, electrical, and structural techniques. In particular, earlier Hall-effect measurements on this sample have demonstrated a world’s record mobility, and the optical and structural properties are also consistent with very high quality. However, it is well known that HVPE GaN/Al$_2$O$_3$ layers always have a thin, degenerate layer in the interface region, and this layer typically has a strong influence on the overall Hall-effect measurements, even at high temperatures. It is possible to correct for the effects of the interface layer, but sometimes the accuracy of the corrections is uncertain. Thus, we have used reactive-ion etching to remove about 30 $\mu$m of material from the N face of our sample, effectively eliminating the degenerate layer and leaving a total thickness of about 220 $\mu$m.

The van der Pauw–Hall-effect measurements were performed with a LakeShore model 7507 apparatus, including a closed-cycle He cooling system operating from 15 to 320 K. Under a heating cycle, the thermometer and sample temperatures differed by only 0.7 K at a nominal temperature of 300 K; even so, a simple, linear temperature correction was implemented to account for this small difference. Thus, temperature accuracy was well within 0.5 K over the whole range. The magnetic field was set at 2 kG, which had a negligible effect on the Hall coefficient $R$ and conductivity $\sigma$, even at the highest mobility, which occurred at about 70 K. (Note that at the more commonly used field of 10 kG, the measured field-induced error in $R$ at 70 K is 3%, and in $\sigma$, 5%. At 300 K, the field-induced error in either is negligible.) From measurements of $R$ and $\sigma$, the Hall mobility $\mu_H = R \sigma$ and the Hall concentration $n_H = 1/eR$ could be calcu-
lated at each temperature. These results are shown in Figs. 1 and 2, respectively. It should be remembered that the conductivity mobility $\mu_c$ is related to the Hall mobility by $\mu_c = \frac{\mu_H}{r}$, where $r$ is the so-called Hall $r$ factor; also, the true carrier concentration $n$ is related to $n_H$ by $n = r n_H$. In practice, $\mu_H$ is of more interest than $\mu_c$, because $\mu_H$ is much easier to measure and thus is a better figure of merit. However, $n$ is of more interest than $n_H$, because $N_D$, $N_A$, and $E_D$ are calculated from the temperature dependences of $n$, not $n_H$; thus, for the highest accuracy, it is necessary to calculate $r$ (discussed below). In Fig. 2, both the raw $n_H$ and the $r$-corrected $n$ values are shown. For this sample, $r = 1.1$–1.2 from 50 to 320 K.

The theoretical fits of $\mu_H$ and $n$ are shown as solid lines in Figs. 1 and 2, respectively. In principle, the fits must be carried out simultaneously, since $\mu_H$ is a function of $n$. A convenient way to implement this process is to first fit $\mu_H$ vs. $T$, with $n = n_H$, and get an approximate set of values for $r$ vs. $T$. Then, a new set of $n$ values can be calculated from $n = r n_H$, and $\mu_H$ vs $T$ can be refitted with the new values of $n$, obtaining a new set of $r$ values. However, it is usually found that the new set of $r$ values differs little from the first set. The mobility is calculated by using an iterative solution of the Boltzmann equation, as developed by Rode.12 We have used Nag’s treatment13 of this method and have included scattering terms arising from optical-lattice modes; deformation-potential and piezoelectric-potential acoustical lattice modes; and ionized impurities and defects, treated in the Brooks–Herring model. We have also included neutral impurity/defect scattering, following Erginsoy’s formulation.14 However, dislocation scattering15 has been ignored, because the measured edge dislocation density on the Ga face is only about $10^3$–$10^4$ cm$^{-2}$. (Further discussion on this matter is presented below.)

The scattering rates depend on various parameters, as follows: polar optical, $\sim (m^* P_{po}(\varepsilon_{o}^{-1} \varepsilon_{0}^{-1})/(\exp(T_{po}/T) - 1)$; acoustic deformation potential, $(m^* \Omega^2 E_1^2/c_L$; acoustic piezoelectric potential, $(m^* \Omega^2 P_{po}/\varepsilon_0$; ionized-impurity/defect, $(2N_A + n)f(n)/(m^* \varepsilon_0^2)$, where $f(n)$ is a weak function of $n$; and neutral impurity/defect, $(N_D - N_A - n)\varepsilon_0/m^*$. In these formulas, $m^*$ is the effective mass, generally accepted16 as 0.22$m_0$; $\varepsilon_0$ and $\varepsilon_{oo}$ are the relative static17 and high-frequency18 dielectric constants, respectively, taken to be $\varepsilon_0 = 10.4$ and $\varepsilon_{oo} = 5.15$, although other values are also commonly used;16,19 $T_{po}$ is the polar-optical temperature, well accepted as $T_{po} = 1057$ K ($= 735$ cm$^{-1} - 91.1$ meV);20 $E_1$ is the acoustic deformation potential (the change of conduction-band energy per unit strain), given in one reference21 as 9.2 eV, for the hydrostatic component, but having no firm consensus;22 $c_L$ is the longitudinal elastic constant, defined for the wurtzite structure by Eq. (104) of Ref. 12, and calculated as $c_L = 3.82 \times 10^{11}$ N/m$^2$ from components of the elastic tensor determined from x-ray measurements;23,24 and $P_{po}$ is the perpendicular component of the piezoelectric coefficient, defined for the wurtzite structure by Eq. (101) of Ref. 12, and given theoretically as $P_{po} = 0.113$ (dimensionless), from theoretical components25 of the piezoelectric tensor $e_{ij}$ (with an assumption that $e_{15} = e_{31}$), and experimental components26 of the elastic tensor $c_{ij}$. Finally, $N_D$, $N_A$, and $n$ (= $rn_H$) are determined from the $n_H$ vs $T$ and $\mu_H$ vs $T$ data.

In the mobility fitting process, we take $m^*$, $\varepsilon_0$, $\varepsilon_{oo}$, and $T_{po}$ as fixed, since the literature values for $m^*$, $\varepsilon_0$, and $\varepsilon_{oo}$ are nowadays consistent within about 10%, and $T_{po}$, within about 2%. However, there is wide uncertainty in the other lattice parameters, $E_1$, $c_L$, and $P_{po}$, so we must fit the quantities $E_1^2/c_L$ and $P_{po}$, along with $N_A$. If we use x-ray values24 of the elastic tensor, then $c_L = 3.82 \times 10^{11}$ N/m$^2$, and our fitted value of $E_1$ becomes 13.5 eV per unit strain; this compares favorably with a hydrostatic value of 9.2 eV, determined from optical measurements.21 Also, our fitted value of $P_{po}$, 0.083, is acceptably close to the theoretical value given above, 0.113. In zinc-blende materials, the piezoelectric scattering strength is often quoted in terms of $e_{15} = \frac{h_{pz}}{(e_{0}\varepsilon_{oo})^{1/2}P_{po}(1 - P_{po}^2)^{1/2}} \approx 0.49$ C/m$^2$, in our case. Finally, the last unknown parameter in the scattering formalism is $N_A$, and here we get $N_A = 1.7 \times 10^{15}$ cm$^{-3}$. Then, from the $n$ vs $T$ data, we can also obtain $N_D = 6.7 \times 10^{15}$ cm$^{-3}$ and $E_D = 25.7$ meV. We believe that the values of $N_D$ and $N_A$ are the smallest obtained in GaN, and $E_D$, the largest, attesting to the high quality of the material. With regard to $E_D$, the donor potential can be screened by free and bound charges, and the effects of the screening are usually modeled by a
The lattice-scattering parameters have then been used in conjunction with the estimated lowest possible values of \(N_D\) and \(N_A\) to determine the maximum values of mobility in bulk GaN, as a function of temperature. The 77 K mobility in the present sample is compatible only with a value of dislocation density \(\rho_D < 10^{12} \text{ cm}^{-2}\), consistent with measured values of \(\rho_D\).

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