8-1-2001

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Predicted maximum mobility in bulk GaN

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(Received 14 May 2001; accepted for publication 22 June 2001)

A 300 K bulk (three-dimensional) mobility of 1245 cm$^2$/V s has been measured in free-standing GaN. Temperature-dependent Hall-effect data on this particular sample are fitted to obtain unknown lattice-scattering parameters, as well as shallow donor ($N_D$) and acceptor ($N_A$) concentrations, which are $N_D = 6.7 \times 10^{15}$ and $N_A = 1.7 \times 10^{15}$ cm$^{-3}$. Realistic values of the maximum mobility attainable in bulk GaN are then obtained by assuming two-orders-of-magnitude lower values of $N_D$ and $N_A$, leading to a maximum 300 K mobility of 1350 cm$^2$/V s, and a maximum 77 K mobility of 19 200 cm$^2$/V s. © 2001 American Institute of Physics. [DOI: 10.1063/1.1394954]

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 $h_{zz}$). 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 $h_{zz}$ 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 at 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-
used Nag’s treatment\textsuperscript{13} of this method and have included scattering terms arising from polar-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.\textsuperscript{14} However, dislocation scattering\textsuperscript{15} 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, $\sim (m^* / P_{oo}) (\varepsilon_0^{-1} - \varepsilon_\infty^{-1}) / [\exp(P_{oo}/T) - 1]$; acoustic deformation potential, $(m^* / E_{ij})^{1/2} / c_L$; and piezoelectric potential, $(m^* / P_{ij})^{1/2} / E_{ij}$; ionized-impurity/defect, $(2N_A + n)f(n)/(m^* / E_{ij})^{1/2}$, 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 accepted as $0.22m_0$; $\varepsilon_0$ and $\varepsilon_\infty$ are the relative static\textsuperscript{17} and high-frequency\textsuperscript{18} dielectric constants, respectively, taken to be $\varepsilon_0 = 10.4$ and $\varepsilon_\infty = 5.15$, although other values are also commonly used;\textsuperscript{16,19} $P_{oo}$ is the polar-optical temperature, well accepted as $P_{oo} = 1057 K ( = 735 \text{ cm}^{-1} = 91.1 \text{ meV})$;\textsuperscript{20} $E_1$ is the acoustic deformation potential (the change of conduction-band energy per unit strain), given in one reference\textsuperscript{21} as 9.2 eV, for the hydrostatic component, but having no firm consensus;\textsuperscript{22} $c_L$ is the longitudinal elastic constant, defined for the wurtzite structure by Eq. (104) of Ref. 12, and calculated as $c_L = 3.82 \times 10^{11} \text{ N/m}^2$ from components of the elastic tensor determined from x-ray measurements;\textsuperscript{23,24} and $P_{ij}$ is the perpendicular component of the piezoelectric coefficient, defined for the wurtzite structure by Eq. (101) of Ref. 12, and given theoretically as $P = 0.113$ (dimensionless), from theoretical components\textsuperscript{25} of the piezoelectric tensor $e_{ij}$ (with an assumption that $e_{15} = e_{31}$), and experimental components\textsuperscript{26} of the elastic tensor $c_{ij}$. Finally, $N_D$, $N_A$, and $n (= n_H)$ are determined from the $n_H$ vs $T$ and $\mu_H$ vs $T$ data.

In the mobility fitting process, we take $m^*$, $\varepsilon_0$, $\varepsilon_\infty$, and $T_{po}$ as fixed, since the literature values for $m^*$, $\varepsilon_0$, and $\varepsilon_\infty$ are nowadays consistent within about 10%, and $T_{po}$, within about 2%. However, there is wide uncertainty in the other lattice parameters, $E_{ij}$, $c_L$, and $P_{ij}$, so we must fit the quantities $E_{ij}^{1/2} / c_L$ and $P_{ij}$, along with $N_A$. If we use x-ray values\textsuperscript{24} of the elastic tensor, then $c_{ij} = 3.82 \times 10^{11} \text{ N/m}^2$, 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.\textsuperscript{21} Also, our fitted value of $P_{ij}$, 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 $e_{ij}^{p,z} = (\varepsilon_0 e_{ij}/c_L) / (1 - P_{ij}^{1/2})^{1/2} = 0.49 \text{ C/m}^2$, in our case. Finally, the last unknown parameter in the scattering formalism is $N_A$, and here we get $N_A = 1.7 \times 10^{15} \text{ cm}^{-3}$. Then, from the $n$ vs $T$ data, we can also obtain $N_D = 6.7 \times 10^{15} \text{ cm}^{-3}$ and $E_{po} = 25.7 \text{ meV}$. We believe that the values of $N_D$ and $N_A$ are the smallest obtained in GaN, and $E_{po}$, the largest, attesting to the high quality of the material. With regard to $E_{po}$, the donor potential can be screened by free and bound charges, and the effects of the screening are usually modeled by a
simple formula, $E_D = E_{D0} - \alpha N_D^{1/3}$. Although the value of $\alpha$ is not well known, one study has suggested $\alpha \approx 2.1 \times 10^{-5}$ meV cm, which would lead to $E_{D0} \approx 30$ meV, in our case. The hydrogenic donor formula, $E_{DH} = 13.6m_e^*/\epsilon_0^2$, would then predict a static dielectric constant $\epsilon_0 = 10.0$, comfortably within the literature range, 9.5–10.4. Thus, our Hall-effect analysis seems to be solidly based in all aspects, and we believe that it can be used to predict mobilities for other values of $N_D$ and $N_A$.

To determine the maximum realistic mobilities, we now set $N_D$ and $N_A$ to the lowest reasonable values. From a comparison with the GaAs case, it would seem possible to reduce $N_D$ and $N_A$ in GaN by perhaps two orders of magnitude to $6.7 \times 10^{13}$ and $1.7 \times 10^{13}$ cm$^{-3}$, respectively, maintaining the compensation ratio measured above. At $N_D = 6.7 \times 10^{13}$ cm$^{-3}$, we would expect $E_D$ to be 29 meV. These values of $N_D$, $N_A$, and $E_D$ then predict the upper curve in Fig. 3. From this curve, $\mu_H = 1350$ cm$^2$/Vs at 300 K, and $\mu_H = 19200$ cm$^2$/Vs at 77 K. Note that the 300 K $\mu_H$ of our present sample, $1245$ cm$^2$/Vs is not too far below the maximum 300 K $\mu_H$. Thus, for very pure samples, the 77 K $\mu_H$ becomes a more definitive figure of merit than the 300 K $\mu_H$.

We have ignored dislocation scattering in the present sample because the measured dislocation density $N_{dis}$ of $10^3$–$10^5$ cm$^{-2}$ will not appreciably affect either its 300 or 77 K mobilities. However, a density of $10^3$ cm$^{-2}$ would have dropped the 300 K $\mu_H$ by about 3%, and the 77 K $\mu_H$ by about 38%. Furthermore, $N_{dis}$ will become even more important as $N_D$ and $N_A$ become smaller. For example, in the pure sample discussed above, an $N_{dis}$ of only $10^2$ cm$^{-2}$ would have dropped the 300 K $\mu_H$ by about 7%, and the 77 K $\mu_H$ by about 59%. It also should be noted that a dislocation density of $10^4$ cm$^{-2}$ provides an effective acceptor density of $10^6/5.185 \times 10^{-8} \approx 2 \times 10^{13}$ cm$^{-3}$, requiring a value $N_D - N_A \approx 2 \times 10^{13}$ cm$^{-3}$ to even have free carriers.

In conclusion, we have fitted the best available GaN sample with an accurate scattering theory, and have determined reasonable values of the various lattice-scattering parameters as well as the donor and acceptor concentrations. 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 $\rho_D < 10^7$ cm$^{-2}$, consistent with measured values of $\rho_D$.

The authors wish to thank S. S. Park and K. Y. Lee of Samsung for growing the sample, C. M. Sung and M. Callahan for helping us obtain it, A. Saxler and H. Morkoç for helpful discussions, and T. A. Cooper for the Hall-effect measurements. One of the authors (D.C.L.) was supported by AFOSR Grant No. F49620-00-1-0347 and U.S. Air Force Contract No. F33615-00-C-5402.