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journal or publication title	Applied physics letters
volume	96
number	252103
page range	1-3
year	2010-06
URL	http://hdl.handle.net/10098/3005

Temperature dependence of electron concentration and mobility in n-GaN measured up to 1020 K

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(Received 8 April 2010; accepted 3 June 2010; published online 22 June 2010)

Temperature dependence of Hall electron concentration and mobility in n-GaN has been measured up to 1020 K. The electron concentration increased monotonically with temperature and did not saturate. The measured values were fitted with the calculated ones for the whole temperature range. It is found that following two assumptions have to be made in order to obtain the best fit for both electron concentration and mobility: (i) two donor levels and one acceptor level (including dislocation) have to be taken into account; and (ii) one donor level lies in the conduction band. The obtained results in this study will contribute to the design of GaN devices operating at high temperatures. © 2010 American Institute of Physics. [doi:10.1063/1.3456560]

Gallium nitride (GaN) is an attractive material for optical and electronic devices. Its wide band gap of 3.4 eV enables to apply GaN to short wavelength (blue) lasers and high breakdown, high temperature operation power transistors/diodes. In order to design these devices, electron/hole concentrations and mobility have to be controlled properly. Intensive studies had been carried out in 1990s on the origin of donor/acceptor levels by theoretical calculations^{1–3} and experimental measurements such as Hall effect,^{4–8} Photoluminescence,⁹ secondary ion mass spectroscopy,¹⁰ optical absorption,¹¹ and Raman scattering.^{12–15} Throughout these works, the origin of shallow donor has been assigned to be as follows: (i) doped silicon (Si) substituting the gallium vacancy,^{5,8} (ii) oxygen substituting the nitrogen vacancy,^{8,9,11,14} and (iii) nitrogen vacancy^{1,10} as the candidates. The energy for these donor levels reported so far are 30–40 meV from the conduction band edge.^{4,5,7–9,15} Shallower donor levels of 12 (Ref. 8) and 20 meV (Ref. 16) are also reported, the latter one is assigned to be hydrogen related. Among them, the most interesting donor level seems to be the nitrogen vacancy related one. Jenkins *et al.*¹ calculated the donor energy level related to nitrogen vacancy and showed that the p-like level lied at 0.6 eV above the conduction band edge, and it was confirmed experimentally by Wetzel *et al.*¹³ Although the understanding on shallow donor levels in GaN has been deepened by these works, almost all the experiments are executed in the temperatures lower than 300 K. The results of higher temperature Hall measurements reported so far are limited to be 400–500 K.^{6,8} In order to obtain deeper understandings on the behavior of electron concentration and mobility, higher temperature measurement is indispensable.

In this letter, electron concentration and mobility are measured in the temperature range from 77 to 1020 K by van der Pauw technique and the results are fitted with the calculated values. It is found that (i) two donor levels and one acceptor level (including dislocation) have to be assumed and (ii) both donor levels are shallow and one of which has to exist in the conduction band; in order to fit measured and calculated results for the whole temperature range.

The used sample in the experiment is an epitaxial layer grown by metal organic chemical vapor deposition method on 3 in. sapphire substrate. After the growth of nucleation buffer layer, Si doped n-type layer with a thickness of 0.5 μm was grown. The doping concentration was nominally $5 \times 10^{17} \text{ cm}^{-3}$. Cutting the wafer with $5 \times 5 \text{ mm}^2$ size, Ohmic metals consisting of Ti/Al/Mo/Au with a thickness of 15/60/35/50 nm, respectively, were evaporated in the four corners to obtain the van der Pauw configuration. The evaporated piece was alloyed at 800 °C for 30 s to ensure good Ohmic contact. The processed sample was set to the Hall measurement system (Toyo technica ResiTest 8310). The measurement was carried out with two steps, that is, first from 77 to 300 K and second from 300 to 1020 K. The applied magnetic field was 0.55 T. Ohmic characteristics were checked for each temperature before the measurement to ensure the measurement reliability and reproducibility. All the measurements could be done with a current of 2 mA and a correlation factor (*f*) of larger than 0.91.

The obtained results were fitted with calculated ones. The fitting was carried out with the following manner. First, the Fermi level position was calculated from the measured electron concentrations. Then, assuming the donor energy level and concentration, the ionized donor concentrations were calculated for the whole temperature range until the best fit was obtained.

The charge neutrality equation for n-type semiconductors is expressed as follows:¹⁷

$$n = N_d^+ - N_a^- - N_{\text{dis}}/c, \quad (1)$$

where *n* is the measured electron concentration, N_d^+ is the ionized donor, N_a^- is the ionized acceptor concentrations, N_{dis} is the dislocation density in cm^{-2} and *c* is the lattice constant along the (0001) direction, respectively.

In Eq. (1), the intrinsic electron concentration was neglected because it was calculated to be $1 \times 10^{10} \text{ cm}^{-3}$ even at 1000 K, which is negligibly small as compared with the measured values. N_d^+ was calculated with the following equation:⁸

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FIG. 1. Temperature dependence of the Fermi level position. Fermi level lies 1.4 meV from the conduction band edge at 77 K and moves toward the forbidden gap with increasing the temperature. It lies 0.26 eV at 1020 K.

$$N_d^+ = \sum_{i=1}^M \frac{N_{di}}{1 + \frac{g_i n}{N_c} \exp\left(\frac{\Delta E_{di}}{kT}\right)}, \quad (2)$$

where the index i refers to the i th donor, M is the number of independent donor level, N_{di} is its concentration, g_i is the degeneracy of its electronic state ($=2$), N_c is the conduction band density of states, ΔE_{di} is the activation energy of the donor electrons, k is the Boltzmann's constant, and T is the absolute temperature, respectively. The acceptor was assumed to be fully ionized throughout the whole temperature because Fermi level was positioned close to the conduction band. Dislocation was assumed to be acceptorlike, that is, negatively charged with trapping the free electrons.^{18–20} The occupancy of electron in the dislocation was assumed to be 1 for the whole temperature range, which seemed to be reasonable considering the calculated results as shown by Wright and Grossner²¹ and Leung *et al.*²²

For calculating the mobility, six scattering mechanisms were taken into account, i.e., ionized impurity, neutral impurity, dislocation, deformation potential (acoustic phonon), piezoelectric, and polar optical phonon scatterings. In the calculation, following parameters were used: electron effective mass $=0.23 m_0$, static and high frequency dielectric constant $=10.4$ and 5.15 , respectively, lattice constant $=5.187 \text{ \AA}$, mass density $=6150 \text{ kg/cm}^3$, sound velocity $=6590 \text{ m/s}$, deformation potential for acoustic phonon $=13.5 \text{ eV}$, polar optical phonon temperature $=1044 \text{ K}$, and piezoelectric constant $=0.5 \text{ C/m}^2$. These values were referred from Ref. 23 except for dielectric constant and deformation potential, which were found in Ref. 7. Calculations were done by the analytical equation cited in Refs. 23 and 20 (for dislocation scattering).

Calculations of electron concentration and mobility were carried out iteratively with assuming the several donor levels/concentrations, acceptor and dislocation concentrations until the sufficient fit was obtained for the whole measured temperature range.

Figure 1 shows the calculated Fermi level position as a function of temperature. As is shown in the figure, Fermi level exists at 1.4 meV below the conduction band edge at 77 K and moves downward monotonically toward the forbid-

FIG. 2. Electron concentration as a function of reciprocal temperature (a) and electron mobility as a function of temperature (b). The open circles show the measured results and the solid lines show the fitted ones. The inset shows the assumed donor, acceptor and dislocation concentrations, and donor energy levels giving the best fit.

den band with increasing the temperature. No Fermi level pinning is observed in the measured temperatures. The Fermi level position at 1020 K is found to be 0.26 eV below the conduction band edge.

Figures 2(a) and 2(b) show the electron concentration as a function of reciprocal temperature and the electron mobility as a function of temperature, respectively. In the figures, the measured values are shown in open circles and fitted ones in solid lines. The donor levels/concentrations, acceptor and dislocation concentrations giving the best fit are also shown in the inset. The fitting is satisfactory with the difference between measured and calculated values being within 7% for electron concentration and 12% for mobility in the whole temperature range. As is shown in Fig. 2(a), electron concentration increases monotonically with temperature and does not saturate even at 1020 K. Notice that the variation in electron concentration with temperature is as small as 2.8 times ($3.1 \times 10^{17} \text{ cm}^{-3}$ at 77 K and $8.7 \times 10^{17} \text{ cm}^{-3}$ at 1020 K), which implies that the donor level is very shallow.

TABLE I. Calculated proportion of total mobility divided by individual mobility for several temperatures. Below 100 K, mobility is almost determined by the ionized impurity ($\mu_{\text{total}}/\mu_{\text{ion}}$) and dislocation ($\mu_{\text{total}}/\mu_{\text{dis}}$) scatterings, while it is dominated by the polar optical phonon ($\mu_{\text{total}}/\mu_{\text{pop}}$) and deformation potential ($\mu_{\text{total}}/\mu_{\text{dp}}$) scatterings in the temperatures over 500 K.

T (K)	$\mu_{\text{total}}/\mu_{\text{ion}}$	$\mu_{\text{total}}/\mu_{\text{dis}}$	$\mu_{\text{total}}/\mu_{\text{dp}}$	$\mu_{\text{total}}/\mu_{\text{pz}}$	$\mu_{\text{total}}/\mu_{\text{pop}}$
100	0.77	0.20	0.01	0.01	1.31×10^{-4}
300	0.52	0.09	0.09	0.02	0.27
570	0.13	0.02	0.10	0.01	0.73
720	0.08	0.01	0.11	0.01	0.79
1020	0.04	0.01	0.13	0.01	0.82

In fact, two donor levels of $N_{d1}=6.8 \times 10^{17} \text{ cm}^{-3}$ with energy level $E_{d1}=-0.4 \text{ eV}$ (minus sign indicates that the donor level exists in the conduction band) and $N_{d2}=9.3 \times 10^{17} \text{ cm}^{-3}$, $E_{d2}=4 \text{ meV}$, acceptor with a concentration of $6.1 \times 10^{17} \text{ cm}^{-3}$, and dislocation density of $5.0 \times 10^8 \text{ cm}^{-2}$ give the best fit. Several donor levels and concentrations are assumed for better fitting, however, it is not satisfactory anyhow to fit with assuming single donor level, nor assuming it in the forbidden band. Therefore, two donor levels of which one lies in the conduction band are considered. The negatively charged acceptor and dislocation concentrations are introduced for adjusting the total impurity concentration in order to explain the mobility behavior, especially at lower temperatures. Without acceptor and dislocation, total impurity concentration is too small to fit with only two donor concentrations. The compensation ratio (N_a/N_d) is about 0.38, which is reasonable as compared with the previously reported values.^{17,20,24} The dislocation density of $5.0 \times 10^8 \text{ cm}^{-2}$ corresponding to $9.6 \times 10^{15} \text{ cm}^{-3}$ in volume (N_{dis}/c) is one order of magnitude smaller than the acceptor concentration. Therefore, it does not affect the electron concentration, however, such a density is required in order to fit the mobility. Look and Molnar²⁴ pointed out that the interfacial layer at GaN/sapphire might cause a falsely donor level in the analysis. For the fitting of the present results, the temperature dependence of electron concentration is too small to explain by assuming interfacial layer and single donor level. Although lower temperature measurement below 30 K may make the existence of interfacial layer clear, it is not available in this study due to the equipment limit. Table I lists the calculated proportion of total mobility divided by individual mobility for several temperatures. In the Table, values of neutral impurity scattering are omitted because its proportion is less than 3×10^{-3} for the whole temperatures. Below 100 K, mobility is almost determined by the ionized impurity ($\mu_{\text{total}}/\mu_{\text{ion}}$) and dislocation ($\mu_{\text{total}}/\mu_{\text{dis}}$) scatterings, while it is dominated by the polar optical phonon ($\mu_{\text{total}}/\mu_{\text{pop}}$) and deformation potential ($\mu_{\text{total}}/\mu_{\text{dp}}$) scatterings in the temperatures over 500 K.

The assumed donor level of -0.4 eV above the conduction band edge coincides with the level originated from the nitrogen vacancy which is theoretically predicted by Jenkins

et al.,¹ and confirmed by Wetzel *et al.*¹³ The origin of the donor level of 4 meV below the conduction band is not clear at present, however, it is plausible that it is nitrogen vacancy related, judging from the previous report,⁶ although the energy level is slightly different. Regarding the mobility, sufficient fit is not obtained with the measured value at 77 K. This may be explained by considering the hopping conduction through the donor bands,⁴⁻⁶ which is not taken into account in this work. Donor level originated from the doped Si having 30–40 meV activation energy is not observed, that is, the experimental results cannot be fitted with assuming such a deeper level.

In conclusion, temperature dependence of electron concentrations and mobility has been measured from 77 to 1020 K. The obtained results are fitted with the calculated ones for whole temperature range. It is found that (i) two donor levels, one ionized acceptor and dislocation have to be taken into account and (ii) one donor level lies in the conduction band; in order to obtain the best fit. The measured electron concentration and mobility behaviors in this work will contribute to the design of GaN devices operating at high temperatures.

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