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Temperature-dependent hole transport in GaN

D Lancefield[1] **and H Eshghi**[2]

[1] Department of Physics, School of Physics and Chemistry, University of Surrey, Guildford, Surrey GU2 7XH, UK
[2] Department of Physics, Shahroud University, Shahroud 316-36155, Iran

E-mail: d.lancefield@surrey.ac.uk

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Abstract

The transport properties of Mg-doped, p-type GaN films grown by MOCVD have been measured using Hall effect and resistivity measurements over a temperature range of 400–120 K. The mobility is found to increase slowly over the temperature range of 400–150 K. Below this temperature the mobility is seen to decrease rapidly, while the corresponding Hall carrier density goes through a minimum before increasing to lower temperatures. These results have been analysed, using a two-band model. This incorporates a simple valence band model, calculated using a relaxation time approximation, and additional transport within an acceptor impurity band. A good fit has been obtained self-consistently to both the mobility and carrier density over a temperature range of 400–120 K. We find that neutral scattering plays an important role in limiting the hole mobility.

1. Introduction

Since the first reports of the successful p-type doping of GaN [1, 2] there has been considerable progress in the development of group III–N materials for electronic and optoelectronic applications. However, the reliable formation of highly-conducting p-type GaN remains a challenge. The Mg acceptor level is typically $\sim$170 meV above the valence band edge so that doping levels of $\sim 10^{20}$ cm^{-3} are often required in devices. To date, the carrier density always exhibits a temperature dependence [3–5] and it has been shown that this can have a significant effect on the operation of some devices [6]. Such high doping levels also lead to the possibility of impurity band formation, while autocompensation may limit the hole mobility and the maximum attainable hole density. Kim *et al* [7] have shown that autocompensation by a Mg_{Ga}–V_N deep donor can be reduced by a nitrogen plasma treatment while Korotkov *et al* [8] found that the room-temperature hole density can be increased by over an order of magnitude by codoping Mg with oxygen. Alternatively, superlattice structures have also been proposed [9].

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Although many researchers have modelled the electron mobility of n-type GaN (see, for example, [10, 11]) there have been relatively few papers describing the hole mobility and undertaking a detailed analysis of its temperature dependence [12–14]. A rigorous analysis is difficult because of the complexity of the valence band structure. Kim *et al* [13] and Cheong *et al* [14] have assumed a parabolic and spherical constant energy surface and have performed a two-band numerical calculation including heavy- and light-hole bands using an iterative technique for solving the Boltzmann equation. In this paper, we report measurements of the transport properties of p-type GaN as a function of temperature. To analyse the results we have adopted a simple two-band model with a single 'effective' valence band and an impurity band. We have analysed the data using the less rigorous relaxation time approximation but we have incorporated neutral impurity scattering which has been ignored previously.

2. Experimental procedure

The Mg-doped samples reported here were all grown by MOCVD on (0001) sapphire. The layers were typically $\sim$1–2 μm thick and were grown on a low-temperature GaN buffer layer. Nominally undoped material grown in the same reactor was typically found to have a background electron concentration of $\sim 10^{17}$ cm^{-3}. In order to activate the Mg acceptors the samples underwent rapid thermal annealing, at 700 °C for 15 min, under an N_2 atmosphere. The samples studied were 6×6 mm^2 squares. Ohmic contacts to the samples were prepared using either evaporated and annealed (5 min at 450 °C) Ni/Au layers or In/Zn alloy dots. Hall effect and resistivity measurements were made over a temperature range of 400–120 K using a Keithley 7605 Hall effect card in high impedance mode. A magnetic field of 0.3 T was used for the Hall measurements. The contacts remained ohmic over the temperature range of the data reported here. The depletion region between the n-type buffer layer and the p-GaN layer under investigation provides electrical isolation. There was no indication that the results were significantly influenced by conduction in the buffer layer.

3. Results and discussions

Figures 1 and 2 show the temperature dependence of Hall hole carrier density p_H $(=1/eR_H)$ and mobility μ_H $(=\sigma R_H)$ for four GaN samples. The hole concentration at room temperature varies from 1.1×10^{17} to 6.5×10^{17} cm^{-3} and the corresponding mobilities vary between 11 and 4 cm^2 V^{-1} s^{-1}. These values are in the same range as those reported elsewhere [3, 4]. The carrier density is seen to decrease exponentially over about three orders of magnitude before going through a minimum between 130 and 150 K. At lower temperatures the Hall carrier density increases while the corresponding mobility drops dramatically. This well known effect is characteristic of carrier transfer to, and conduction within, an impurity band. In this case the measured carrier density and mobility depends on the density and mobility of the carriers in the two bands. For the case of low magnetic fields and assuming that the Hall scattering factors are equal to unity, it can be shown [15] that

$$p_H = \frac{(p_V\mu_V + p_{IB}\mu_{IB})^2}{p_V\mu_V^2 + p_{IB}\mu_{IB}^2} \tag{1}$$

and

$$\mu_H = \frac{p_V\mu_V^2 + p_{IB}\mu_{IB}^2}{p_V\mu_V + p_{IB}\mu_{IB}} \tag{2}$$

where 'V' refers to the valence band and 'IB' refers to the acceptor impurity band.

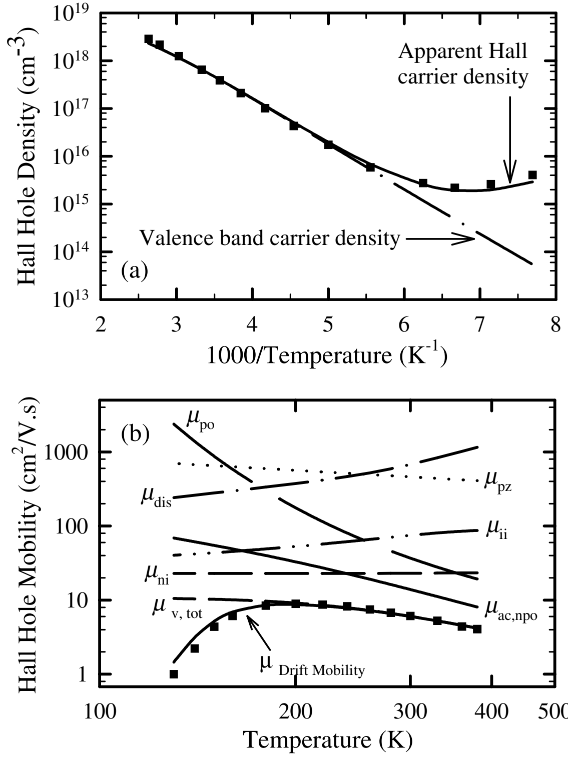

Figure 1. Temperature dependence of (a) hole carrier density and (b) hole mobility determined from Hall effect and resistivity measurements on sample A. The curves show the temperature dependence of the theoretical carrier density or mobility as described in the text.

The carrier density and mobility data were fitted self-consistently although we describe below the analysis of the two measured quantities separately for clarity. For temperatures above 200 K it is reasonable to assume that transport within the valence band dominates for these samples. To analyse the Hall carrier density data we have used the standard expression

$$\frac{p(p+N_d)}{N_a - p - N_d} = \frac{N_V}{g_a} \exp\left(\frac{-\Delta E_a}{k_B T}\right) \tag{3}$$

where N_a and N_d are the acceptor and donor densities, ΔE_a is the activation energy of the acceptor impurity, g_a is the degeneracy factor for acceptor states which we set equal to 4, and N_V is the effective valence band density of states given by

$$N_V = 2(2\pi m_h^* kT)^{3/2}/h^3.$$

The hole effective mass, m_h^*, is not well known. Kim *et al* [13] use values for transverse and longitudinal components of the light- and heavy-hole masses. Here we have used a density of states effective mass of $1.6m_0$. In figure 1(a) the best fit is shown by the dot-dashed curve. Values for the acceptor binding energies obtained from fitting the data shown in figures 1 and 2 are given in table 1.

The analysis of the carrier density alone only allows $N_a - N_d$ to be estimated. However, it is possible to estimate the carrier density in an impurity band from an equation of the form $p_{IB} = P_0 - p_V$, where $P_0 = (1-\theta)N_a$ and θ is the compensation ratio (N_d/N_a). This has been shown to work well for n-type GaN where the low-temperature carrier density often increases before becoming constant at temperatures below 50 K [11]. In this way the carrier density results can provide some guide to the degree of compensation. In p-type GaN we are

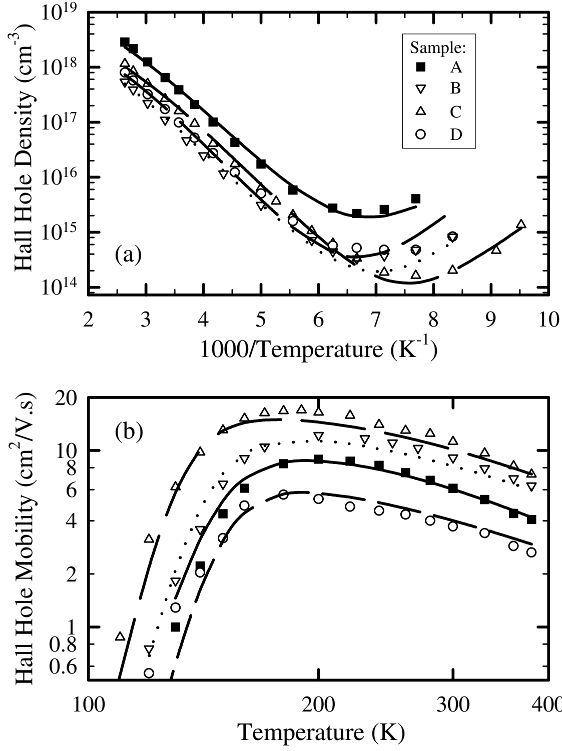

Figure 2. Temperature dependence of (a) hole carrier density and (b) hole mobility of four samples. The curves indicate the best fits to the apparent carrier density and mobility using equations (1) and (2).

Table 1. The best fit parameters for samples, shown in figures 1 and 2.

Sample ID	N_a (cm^{-3})	ΔE_a (meV)	E_{AC} (eV)	Compensation ratio θ
A	1.04×10^{20}	165	20	0.026
B	8.90×10^{18}	166	18	0.013
C	2.33×10^{19}	175	16	0.035
D	1.84×10^{19}	180	30	0.052

not aware of any such low-temperature data. Consequently, we have estimated N_a and N_d by simultaneously fitting the valence band carrier density and mobility as we describe later.

The hole mobility in an impurity band can be estimated using a model described by Shklovskii and Efros [16]

$$\mu_{IB} = \frac{1}{\rho_0 e p_{IB}} \exp\left(\frac{-\Delta E_{hop}}{k_B T}\right) \tag{4}$$

where ρ_0 is the resistivity at $T^{-1} = 0$ and ΔE_{hop} is the hopping activation energy in this band. Using such a model we estimate the impurity band hole mobility to be $\sim 10^{-4}$ cm^2 V^{-1} s^{-1}. An alternative approach assumes that where the Hall carrier density is a minimum the conductivity of the holes in the valence band equals that of the holes in the impurity band. From the data of Kozodoy *et al* [12] and the results shown here it is possible to estimate that an increase in impurity band carrier density of between 10^4 and 10^6 can cause the conductivity of the impurity band to increase to match that of the valence band. The measured hole mobilities range between 10 and 100 cm^2 V^{-1} s^{-1} in the appropriate temperature range. This then suggests that the impurity

band hole mobility should be about 10^{-4}–10^{-3} cm^2 V^{-1} s^{-1}. These very low values might be considered reasonable given that a large hole mass causes a reduction of the overlap of the wave-function between adjacent impurities and the apparently low compensation in these samples.

For the analysis of the hole mobility within the valence band we have used the relaxation time approximation including polar-optical (μ_{po}) and non-polar-optical phonon scattering, acoustic deformation ($\mu_{ac,npo}$), piezoelectric (μ_{pz}), ionized (μ_{ii}) and neutral (μ_{ni}) impurity scattering as described by Wiley [17], and dislocation scattering (μ_{dis}) [18]. Previously Cheong *et al* [14] have included space charge scattering but have ignored neutral impurity scattering. We believe that neutral impurity scattering is quite important because of the large acceptor activation energy. Our analysis is less rigorous than Cheong *et al* but while the uncertainty in many of the material parameters continues a simpler model may still provide some useful insights. For example, hole effective masses between $0.8m_0$ and more recently $1.6m_0$ have been reported [12, 19]. In this analysis the deformation potential (E_{AC}), acceptor density (N_a), their activation energy (ΔE_a), compensation ratio (θ), and dislocation density (N_{dis}) in the material are considered as the fitting parameters. The remaining material parameters used in the analysis are taken from the literature and given in table 2.

Table 2. GaN material parameters.

Parameter	Symbol (units)	Values
Hole effective mass	m_h^*/m_0	1.6
Low-frequency dielectric constant	ε_s	9.9
High-frequency dielectric constant	ε_∞	5.8
Deformation potential ratio	E_{npo}/E_{AC}	1.7
Longitudinal optical phonon temperature	θ (K)	1044
Mass density	ρ_M ($\times 10^{-3}$ kg m^{-3})	6.1
Sound velocity	s ($\times 10^{-3}$ m s^{-1})	6.59
Average longitudinal elastic constant	C_l ($\times 10^{12}$ dyne cm^{-2})	2.65
Average transverse elastic constant	C_t ($\times 10^{11}$ dyne cm^{-2})	4.42
Piezoelectric constant	$(h_{14})^2(3/C_l + 4/C_t)$ ($\times 10^3$ V^2 dyne^{-1})	18.3

Figure 1(b) shows the various scattering components involved in fitting the hole mobility data. $\mu_{V,tot}$ gives the total mobility for holes in the valence band. The agreement with experiment for temperatures above 200 K is good. It is clear that neutral impurity scattering is important in this sample and that the analysis is not very sensitive to the dislocation density. In figure 1(a) the full curve shows the apparent hole carrier density as a function of temperature using equation (1). In figure 1(b) $\mu_{Drift\ Mobility}$ shows the total mobility as a function of temperature using equation (2). We obtained the fits shown with $N_a = 1.0 \times 10^{20}$ cm^{-3}, $\Delta E_a = 165$ meV, $\theta = 0.026$, and $E_{AC} = 20$eV. The fits to the three other samples obtained in a similar way are shown in figure 2. The best-fit parameters are given in table 1. It is clear from these figures that by considering conduction within the acceptor impurity band, in addition to the valence band, allows good fits to experimental data to be obtained over a wide temperature range. The slightly reduced mobility of sample D results in our analysis in a larger deformation potential. It is possible to fit that data with a constant deformation potential if space charge scattering is introduced.

We also performed a similar self-consistent analysis but with different values for the valence band effective mass. For a smaller values we obtained a relatively poor fit to the mobility. This is because a larger acceptor density is necessary to obtain the room-temperature hole density. This increase in acceptors increases impurity scattering, which decreases the mobility and makes it quite temperature independent even at temperatures close to room temperature. Using a density of states effective mass of $1.6m_0$ reduces the role of impurity scattering relative to other scattering mechanisms. No significant improvement could be obtained using a higher hole mass.

4. Conclusions

We have analysed the hole transport properties of a number of p-type GaN epitaxial layers using a self-consistent approach. The analysis uses a two-band model including conduction within a single 'effective' valence band and an acceptor impurity band using a basic relaxation time approximation. We have found that good agreement can be obtained provided neutral impurity scattering is included. For most of our samples a deformation potential of about 20 eV is used. We have estimated the impurity band limited mobility to be $\sim 10^{-4}$ cm^2 V^{-1} s^{-1} in our samples.

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