

## Appendix A: Calculation of band parameters

The valence band of wurtzite GaN is split into three, namely, heavy hole (hh) band, light hole (lh) band and crystal-field split-hole (ch) band.<sup>[28]</sup> The effective mass for the density of states  $m_{\text{Xh}}^{\text{dos}}$  and the effective mass  $m_{\text{Xh}}^*$  in each band (Xh represents hh, lh or ch) is given by

$$m_{\text{Xh}}^{\text{dos}} = (m_{\text{Xh}}^{\parallel} \times m_{\text{Xh}}^{\perp} \times m_{\text{Xh}}^{\perp})^{1/3}, \quad (\text{A1})$$

$$\text{and } m_{\text{Xh}}^* = 3 \left( \frac{1}{m_{\text{Xh}}^{\parallel}} + \frac{1}{m_{\text{Xh}}^{\perp}} + \frac{1}{m_{\text{Xh}}^{\perp}} \right)^{-1}, \quad (\text{A2})$$

where  $m_{\text{Xh}}^{\parallel}$  and  $m_{\text{Xh}}^{\perp}$  represent the components of the hole effective mass in the  $k_z$  direction and in the  $k_x k_y$  plane, respectively.

Therefore, the effective mass for the density of states in valence band,  $m_{\text{h}}^{\text{dos}}$  considering the occupation probability of each band can be expressed by

$$m_{\text{h}}^{\text{dos}} = \left[ (m_{\text{hh}}^{\text{dos}})^{3/2} + (m_{\text{lh}}^{\text{dos}})^{3/2} \times \exp\left(-\frac{\Delta_2}{kT}\right) + (m_{\text{ch}}^{\text{dos}})^{3/2} \times \exp\left(-\frac{\Delta_1}{kT}\right) \right]^{2/3}, \quad (\text{A3})$$

where  $\Delta_1 = \Delta_{\text{cr}}$  is the crystal-field splitting and  $\Delta_2 = 1/3\Delta_{\text{so}}$  ( $\Delta_{\text{so}}$  is spin-orbit splitting).

The effective density of state of valence band  $N_{\text{V}}$  is expressed by

$$N_{\text{V}} = 2(2\pi m_{\text{h}}^{\text{dos}} kT/h^2)^{3/2}. \quad (\text{A4})$$

And, acceptor degeneracy factor  $g$  is obtained by summing over the degeneracy factors (each being 2) of individual bands weighted with the appropriate Boltzmann factors giving

$$g = 2 \times \left[ 1 + \exp\left(-\frac{\Delta_2}{kT}\right) + \exp\left(-\frac{\Delta_1}{kT}\right) \right]. \quad (\text{A5})$$

The influence of three valence bands is again considered. The proportion of holes in each band is related to the effective density of state and the occupation probability. Therefore,  $m_{\text{h}}^*$  is expressed as

$$m_{\text{h}}^* = \frac{m_{\text{hh}}^* \times (m_{\text{hh}}^{\text{dos}})^{3/2} + m_{\text{lh}}^* \times (m_{\text{lh}}^{\text{dos}})^{3/2} \times \exp\left(-\frac{\Delta_2}{kT}\right) + m_{\text{ch}}^* \times (m_{\text{ch}}^{\text{dos}})^{3/2} \times \exp\left(-\frac{\Delta_1}{kT}\right)}{(m_{\text{hh}}^{\text{dos}})^{3/2} + (m_{\text{lh}}^{\text{dos}})^{3/2} \times \exp\left(-\frac{\Delta_2}{kT}\right) + (m_{\text{ch}}^{\text{dos}})^{3/2} \times \exp\left(-\frac{\Delta_1}{kT}\right)}. \quad (\text{A6})$$

All the band parameters above are calculated based on 3D fit values reported by Yeo *et al.*<sup>[28]</sup> and listed in Table A-1.

Table A-1. Band parameters calculated based on 3D fit values in Ref. 28.

$m_{\text{hh}}^*$	$m_{\text{lh}}^*$	$m_{\text{ch}}^*$	$m_{\text{h}}^*$	$m_{\text{hh}}^{\text{dos}}$	$m_{\text{lh}}^{\text{dos}}$	$m_{\text{ch}}^{\text{dos}}$	$m_{\text{h}}^{\text{dos}}$	$N_{\text{V}}$	$g$
$(m_0)$	$(m_0)$	$(m_0)$	$(m_0)$	$(m_0)$	$(m_0)$	$(m_0)$	$(m_0)$	$(\text{cm}^{-3})$	
1.90	0.20	0.37	<b>1.65</b>	1.90	0.34	0.81	<b>2.13</b>	$7.78 \times 10^{19}$	<b>4.62</b>