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A theoretical study of electronic and optical properties in wurtzite GaN

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Abstract. The band structures of wurtzite GaN (α-GaN) are studied using the nearest- and second-nearest-neighbour semi-empirical tight-binding method in the sp^3s^* model. The calculated fundamental direct gap of α-GaN is 3.45 eV. The density of states and the imaginary part of dielectric function ($\epsilon_2(\omega)$) are researched in the region -10.0–12 eV and 0.0–10.0 eV respectively. There are mainly three peaks at 6.4, 7.5 and 8.4 eV, dominating the $\epsilon_2(\omega)$ spectrum. The real part of dielectric function, reflectivity, absorption coefficient and refractive index are all studied.

The development in the past decade of light-emitting diodes and semiconductor lasers operating in the red to green spectral region and the aim to realize full-colour display systems has prompted the search for devices operating in the blue/ultraviolet (UV) energy range. GaN, especially, wurtzite GaN (α-GaN), is a promising candidate for the fabrication of such devices, since it possesses a direct gap in the near UV (around 3.4 eV), is resistant to radiation damage, and can form solid solutions with InN and AlN, which permits the tailoring of its optical and electrical behaviour [1]. The latest applications of α-GaN in optical and microelectronics structures involve device-quality contacts [2], UV photoconductors [3], InGaN/GaN and AlGaN/GaN double-heterostructure UV/blue LEDs [4] etc. The making of these devices is much based on the profound research on α-GaN.

Due to the greater complexity of wurtzite than zinc-blende GaN (β-GaN), until recently, there have been relatively few theoretical studies of α-GaN [5–8], and among those few theoretical studies the most part were only to calculate band structures; other properties of α-GaN are seldom considered. In this work, we present the optical properties as well as band structures of α-GaN using a semi-empirical tight-binding approach (SETB) in the sp^3s^* model.

There are two anions (nitrogen) and two cations (gallium) in the α-GaN unit cell. We adopt the semi-empirical tight-binding theory developed by P Vogl *et al* [9], considering the nearest- and second-nearest-neighbour interactions. An sp^3s^* basis centred at each of the four atomic sites per unit cell is used, which leads to a 20×20 Hamiltonian. The number of non-zero tight-binding parameters are limited to one-centre on-site integrals, nearest- and second-nearest-neighbours two-centre integrals, as discussed by Slater and Koster [10]. For the second-nearest neighbours, only interactions between s^* orbital and three p orbitals are considered. Thus our model has fifteen independent parameters: the six on-site matrix elements $E(\mathrm{s,a})$, $E(\mathrm{s^*,a})$, $E(\mathrm{p,a})$, $E(\mathrm{s,c})$, $E(\mathrm{s^*,c})$ and $E(\mathrm{p,c})$ (where s and p refer to the

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basis states and a and c refer to anion (N) and cation (Ga)), the seven nearest-neighbour transfer matrix elements $V(ss\sigma)$, $V(sp\sigma)$, $V(ps\sigma)$, $V(pp\pi)$, $V(pp\sigma)$, $V(s^*p\sigma)$ and $V(ps^*\sigma)$ (where the first (second) index refers to the N (Ga)), finally, two second-nearest-neighbour transfer matrix elements $V(s^*p, a)$, $V(s^*p, c)$. All these parameters are determined by fitting the band structures with theoretical calculation [8] and experiment [11].

Table 1. The fitted nearest- and second-nearest-neighbour tight-binding parameters of α-GaN in eV.

E(s, a)	E(s*, a)	E(p, a)	E(s, c)	E(s*, c)	E(p, c)	$V(ss\sigma)$	
12.86	3.437	7.603	−1.059	10.17	0.0028	5.660	
$V(sp\sigma)$	$V(ps\sigma)$	$V(pp\pi)$	$V(pp\sigma)$	$V(s^*p\sigma)$	$V(ps^*\sigma)$	$V(s^*p, a)$	$V(s^*p, c)$
6.394	2.945	3.468	−1.594	4.889	−2.522	−0.2217	0.2122

Table 2. Calculated critical-point energies of the major electronic transitions up to 9 eV of α-GaN, according to the most reliable band-structure data found in the literature. The corresponding energies of the experimental dielectric-function structures are also noted.

	Energy (eV)				
Transition	(SETB) This work	(OLCAO)[a] [5]	(LMTO-LDA)[b] [12]	(OLCAO)[c] [13]	(experiment)[d] [11]
Γ_6–Γ_1	3.45	3.50	3.44	2.65	3.35
Γ_5–Γ_3	6.0	5.8	6.0	6.0	
M_4–M_1	6.03	7.05	7.03	6.7	7.0
M_4–M_3	7.2	7.3	7.4	7.25	7.0
H_3–H_3	7.8	8.4	8.8	8.5	7.9
M_2–M_1	8.6	8.5	8.7	8.6	7.9
K_2–K_3	8.0	9.05	9.5	9.0	9.0

[a] Orthogonalized linear combination of atomic orbitals with LDA adjustment [5].
[b] Linear muffin-tin orbital method, with LDA adjustment [12].
[c] Orthogonalized linear combination of atomic orbitals without LDA adjustment [13].
[d] α-GaN thin films grown on sapphire substrate, at room temperature [11].

The fifteen fitted tight-binding parameters are listed in table 1. The fundamental gap of the high-symmetry points in the first Brillouin zone (BZ) are shown in table 2, compared with previously reported band structures (Huang and Ching [5], Logothetidis and Petales [11], Gorczyca and Christensen [12], and Xu and Ching [13]). (The 'transition' in table 2 refers to the band transition energy between the upper valence and lower conduction bands.) The results of them are in agreement each other. Our fundamental gap of Γ is 3.45 eV, which is in good agreement with the experimental data [14]. Figure 1 shows the α-GaN tight-binding structure obtained by our fitting procedure.

As in nearly all tight-binding models, the valence bands in figure 1 are reproduced accurately, which are mainly derived from the N 2p state with a sizable mixture of Ga 4s and 4p states. The lowest conduction band is also well reproduced and is composed primarily of the Ga 4s state. The upper conduction bands are primarily of Ga 4p character and are less accurately reproduced. Fortunately, these are the least important bands in problems concerning the band transition.

From the band structure, the DOS has been obtained by a numerical method developed by Gilat and Raubenheimer [15]. The method involves dividing the irreducible section of

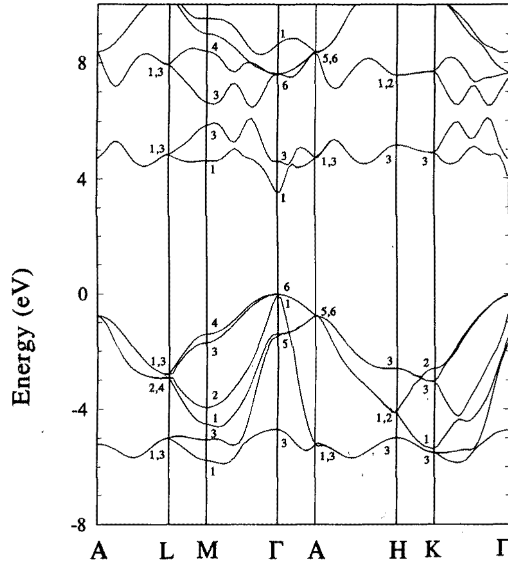

Figure 1. The band structure of α-GaN in the present semi-empirical tight-binding model. The energy zero point is chosen to be at the valence band maximum.

the first BZ into a cubic mesh and approximating the constant-energy surfaces inside every small cube by a set of parallel planes; and perturbation is used to calculate the gradient of equal-energy surface. We used 3552 K points in the irreducible part of the BZ. The results are given in figure 2, where the energy region covers -10–12 eV. Compared with the results of Huang [5] shown in the inset of figure 2, both spectra have the same principal peaks in the corresponding regions, although the positions and heights of the peaks are not in complete agreement. The figure also shows that the direct band gap of α-GaN is about 3.45 eV.

At low temperature, dielectric function of non-polar crystal is determined mainly by the transition beween the valence and conduction bands. According to perturbation theory, $\epsilon_2(\omega)$ is expressed [16]:

$$\epsilon_2(\omega) = \frac{4\pi^2 e^2}{3m^2\omega^2} \sum_{l,n} \int_{BZ} \frac{2}{(2\pi)^3}\, \mathrm{d}^3k |P_{nl}|^2 \delta[E_l(k) - E_n(k) - \hbar\omega] \qquad (1)$$

where m and e are the mass and electrical charge of electron respectively; $\sum_{l,n}$ means summation between the all conduction bands (l) and valence bands (n); and P_{nl} expresses the momentum matrix element between l and n.

Using the tight-binding representation of the optical matrix elements derived by Lew Yan Voon and Ram-Mohan [17], we directly calculate P_{nl} by the K-space Hamiltonian with the fifteen tight-binding parameters. When calculating the integration of $\epsilon_2(\omega)$, we use the same method as used for the DOS. The calculation has been performed in the energy region 0.0–10 eV; and four conduction bands and three valence bands are involved.

The real part of dielectric function($\epsilon_1(\omega)$) can be derived from $\epsilon_2(\omega)$ by the Kramers–Kronig relation. In our calculation the relation is written as the following:

$$\epsilon_1(\omega) - 1 = \frac{2}{\pi} \lim_{\eta\to 0}\left[\int_0^{\omega-\eta} \frac{\omega'\epsilon_2(\omega')}{\omega'^2 - \omega^2}\, \mathrm{d}\omega' + \int_{\omega+\eta}^{\omega_c} \frac{\omega'\epsilon_2(\omega')}{\omega'^2 - \omega^2}\, \mathrm{d}\omega'\right] + \frac{2}{\pi}\int_{\omega_c}^{\infty} \frac{\omega'\epsilon_2(\omega')}{\omega'^2 - \omega^2}\, \mathrm{d}\omega' \qquad (2)$$

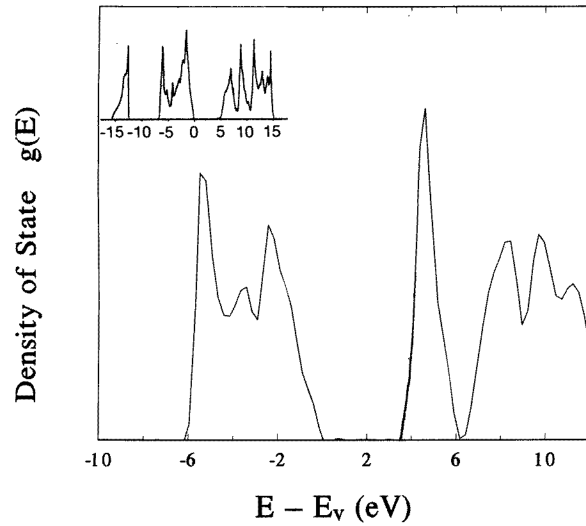

Figure 2. The total DOS for bulk α-GaN, compared with the result of Huang and Ching [5] (the inset).

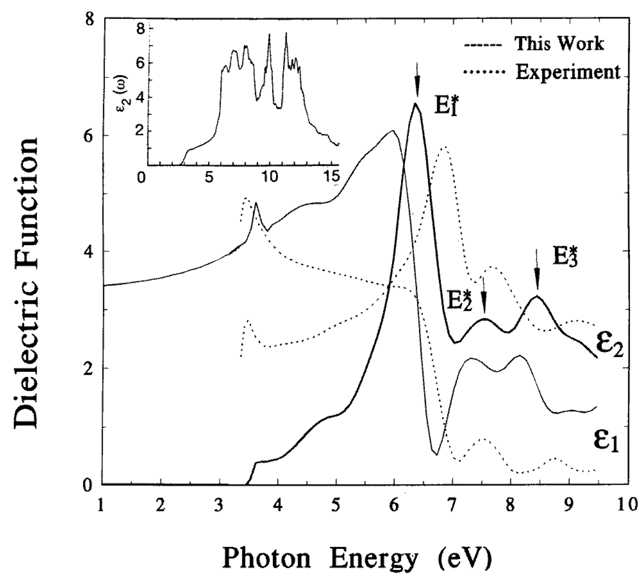

Figure 3. The real (ϵ_1) and imaginary (ϵ_2) parts of the dielectric function of α-GaN, compared with the experimental data. The inset is the result of Christensen and Gorczyca [18].

where η and ω_c (E_c) are 0.0013 and 10.0 eV respectively. When $\omega \geqslant \omega_c$, we take the following approximation: $\epsilon_2(\omega) \approx A/\omega^2$, where constant A is obtained by $\epsilon_2(\omega_c)$: $A = \omega_c^2 \epsilon_2(\omega_c)$. So the last term in (2) is therefore:

$$\frac{2A}{\pi} \int_{\omega_c}^{\infty} \frac{\mathrm{d}\omega'}{(\omega')(\omega'^2 - \omega^2)} = -\frac{\omega_c^2 \epsilon_2(\omega_c)}{\pi \omega^2} \ln\left(1 - \frac{\omega^2}{{\omega_c}^2}\right). \tag{3}$$

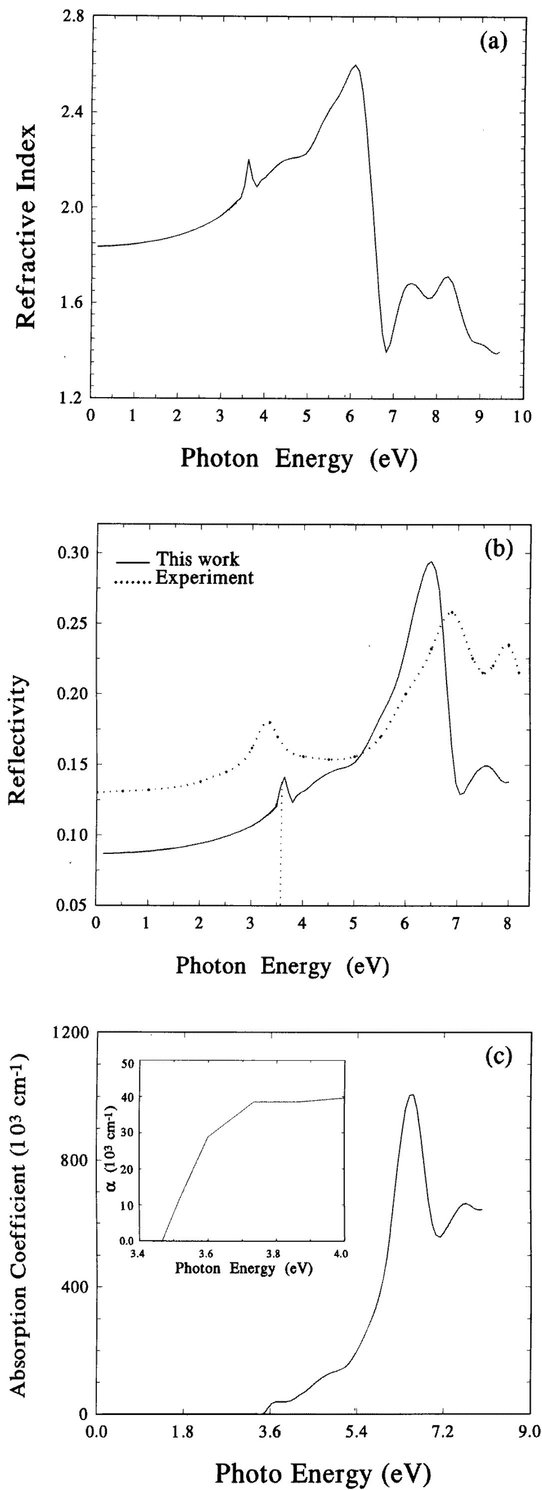

Figure 4. The optical constants of α-GaN: (a) refractive index; (b) reflectivity, compared with experiment by Logothetidis and Petalas [11]; (c) absorption coefficient. The inset is the enlarged picture from 3.4 eV to 4.0 eV.

Figure 3 shows our calculated results of the imaginary and real part of the dielectric function, compared with the experimental data, (which is the unique one, to our knowledge). The inset is $\epsilon_2(\omega)$ calculated by Christensen *et al* [18], using the self-consistent linear muffin-tin-orbital (LMTO) method. In the 1.0–10.0 eV photo energy range, there are three main peaks in our calculation at 6.4, 7.5 and 8.4 eV, denoted E_1^*, E_2^* and E_3^*, respectively in figure 3. And the experimental data is 7.0, 7.9 and 9.0 eV (see table 2). The three peaks of Christensen *et al* are located at 6.1, 6.9 and 7,9 eV.

Referring to table 2, the three distinct structures E_1^*, E_2^* and E_3^* can be assigned to the transition of the specific points in the BZ. The transitions energy of Γ_5–Γ_3 is around 6.0 eV and M_4–M_1, occurs at energies between 6.03 eV and 7.05 eV, obtained by different researchers. These two interband excitations along the Γ–Σ–M line are thought to compose the first structure (E_1^*, 6.4 eV). The second structure (E_2^*, 7.5 eV) could be related to the (M_4–M_3) transition, which is reported to take place from 7.0 eV to 7.4 eV, and possibly to the H point (H_3–H_3) that covers a broad energy region from table 2. The gap of M_2–M_1 and K_2–K_3 direct gap are close to 8.4 eV, so they may be responsible for the third feature (E_3^*, 8.4 eV).

Very important optical constants including the refractive index (n), reflectivity (R) and absorption coefficient (α) are shown in figure 4. Due to the peak at 3.45 eV of $\epsilon_2(\omega)$ and the relation between n, R and $\epsilon_2(\omega)$, one can conclude that there are also peaks of n and R near 3.45 eV, which have been observed in the figure of n and R. Among those optical constants, only R has ever been discussed by previous researchers [11] (see the dotted curve in figure 4(b)). The highest peak of α reaches 1000×10^3 cm^{-1}. The inset of figure 4(c) is the enlarged picture in the range of 3.4–4.0 eV, namely near the band edge. From 3.46 eV to 3.60 eV, α increased steeply by 3.0×10^4 cm^{-1}, which can be interpreted by the direct fundamental gap at the Γ point of α-GaN. This feature of an abrupt limit of absorption energy at lower energy area is very important to the application of photoelectronic device.

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