

Theoretical Study of Electronic Properties of the Semi-Conductors AlN and GaN With the Empirical Pseudopotential Method EPM

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Abstract

The electronic structure of binary compounds AlN and GaN are presented. We have used the empirical pseudo-potential method. Good agreement between the calculated results and experiment is obtained. The charge densities are presented for the sum of the four valence bands of both AlN and GaN.

Key Words: Empirical Pseudo-potential Method (EPM), nitride aluminium, nitride gallium compounds, III-N semi-conductors, wide band gap semi-conductors, energy gap, charge density.

1. Introduction

Wide-energy gap III–V nitride semiconductors GaN and AlN have received considerable attention in both experiment [1–2] and theory [3–4], for their device applications in blue and ultraviolet wavelengths. A number of reviews on GaN and AlN have been given by Strite and Morkoc [5], P. Kung and M. Razegui [6] and Pankove [7]. The vast majority of research on III–V nitride has been focused on the wurtzite crystal phase. The reason is: most III–V nitrides have been grown on sapphire substrates, which generally transfer their hexagonal symmetry to the nitride film. Nevertheless, interest in zincblende nitrides has been growing recently. The zinc-blende GaN has a higher saturated electron drift velocity and a somewhat lower energy band than wurtzite GaN. Mizuta [8] first reported bulk zinc-blende GaN grown on (001) GaAs. There have been several recent studies of the zinc-blende GaN [9–11] and AlN in zinc-blende structures has an indirect gap at 5.11 eV [12]; while zinc-blende GaN with direct gap give us the value of 3.5 eV, as reported by Bloom.

The empirical pseudo-potential method is simple and expected to give quick and reasonably reliable results. However, in the literature, there is a lack of zinc-blende GaN and AlN experimental data regarding the band structures and it is hard to extract empirical form factor parameters for the EPM calculation.

In our work, we adjust the EPM parameters by fitting the band energies of AlN and GaN, obtained using the quasi-particle calculation. Then we use these EPM parameters and the method in References [13–14] to calculate the band structure of zinc-blende GaN and AlN.

2. Calculations

We start with the effective one-electron crystal Hamiltonian [15] using the following relations:

$$H = \frac{p^2}{2m_0} + V_c(\vec{r}); \quad V_c(\vec{r} + \vec{R}) = V_c(\vec{r}) \quad (1)$$

$$H\psi_{n,k}(r) = E_{n,k}\psi_{n,k}(r) \quad (2)$$

$$H_{n,k}(r) = \sum_{\mathbf{G}} a_{n,k}(\mathbf{G}) u_{\mathbf{G},k}, \quad u_{\mathbf{G},k} = \frac{1}{\sqrt{\Omega}} e^{i(\mathbf{G}+\mathbf{k})\cdot r} \quad (3)$$

$$H = \frac{1}{\sqrt{\Omega}} \sum_{\mathbf{G}} a_{n,k}(\mathbf{G}) e^{i(\mathbf{G}+\mathbf{k})\cdot r}. \quad (4)$$

Here, H denotes the effective potential, V_c is the direct lattice vector, and \mathbf{G} denotes the reciprocal lattice vectors. The reciprocal and direct lattice vectors are related via the following:

$$\mathbf{G}\cdot\mathbf{R}=2\pi n, \quad n \in \mathbb{Z}$$

$$H \sum_{\mathbf{G}} a_{n,k}(\mathbf{G}) u_{\mathbf{G},k} = E_{n,k} \sum_{\mathbf{G}} a_{n,k}(\mathbf{G}) u_{\mathbf{G},k} \quad \text{Project this to } u_{\mathbf{G}',k} \quad (5)$$

$$\sum_{\mathbf{G}} a_{n,k}(\mathbf{G}) \int u_{\mathbf{G}',k}^* H u_{\mathbf{G},k} d\tau = \sum_{\mathbf{G}} a_{n,k}(\mathbf{G}) E_{n,k} \int u_{\mathbf{G}',k}^* u_{\mathbf{G},k} d\tau \quad (6)$$

$$\int u_{\mathbf{G}',k}^* H u_{\mathbf{G},k} d\tau = H_{\mathbf{G}',\mathbf{G}(k)}, \quad \int u_{\mathbf{G}',k}^* u_{\mathbf{G},k} d\tau = \Omega \delta_{\mathbf{G},\mathbf{G}'} \quad (7)$$

and

$$\int u_{\mathbf{G}',k}^* u_{\mathbf{G},k} d\tau = \Omega \delta_{\mathbf{G},\mathbf{G}'}. \quad (8)$$

The relation $\Omega \delta_{\mathbf{G},\mathbf{G}'}$ denotes crystal volume. This results in an eigenvalue equation for each value of k :

$$\sum_{\mathbf{G}} a_{n,k}(\mathbf{G}) H_{\mathbf{G}',\mathbf{G}(k)} = \sum_{\mathbf{G}} a_{n,k}(\mathbf{G}) E_{n,k} \delta_{\mathbf{G}',\mathbf{G}}. \quad (9)$$

As this is an infinite set, we hence truncate the matrix size to N reciprocal lattice vectors (RLV):

$$H_{\mathbf{G}',\mathbf{G}} = \frac{1}{\Omega} \int e^{-i(\mathbf{G}'+\mathbf{k})\cdot r} \left(-\frac{\hbar^2}{2m_0} \nabla^2 \right) e^{i(\mathbf{G}+\mathbf{k})\cdot r} d\tau + \frac{1}{\Omega} \int e^{-i(\mathbf{G}'+\mathbf{k})\cdot r} V_c e^{i(\mathbf{G}+\mathbf{k})\cdot r} d\tau, \quad (10)$$

$$H_{\mathbf{G}',\mathbf{G}} = \frac{\hbar^2}{2m_0\Omega} \int |\mathbf{G} + \mathbf{k}|^2 e^{i(\mathbf{G}-\mathbf{G}')\cdot r} d\tau + \frac{1}{\Omega} \int e^{-i(\mathbf{G}'+\mathbf{k})\cdot r} V_c e^{i(\mathbf{G}+\mathbf{k})\cdot r} d\tau; \quad (11)$$

and we make the observation and assignments

$$\frac{\hbar^2}{2m_0\Omega} \int |\mathbf{G} + \mathbf{k}|^2 e^{i(\mathbf{G}-\mathbf{G}')\cdot r} d\tau = \delta_{\mathbf{G}',\mathbf{G}}, \quad (12)$$

$$\frac{1}{\Omega} \int e^{-i(\mathbf{G}'+\mathbf{k})\cdot r} V_c e^{i(\mathbf{G}+\mathbf{k})\cdot r} d\tau = V. \quad (13)$$

Hence, we get this diagonal for the kinetic energy contribution:

$$H_{\mathbf{G}',\mathbf{G}} = \frac{\hbar^2}{2m_0} |\mathbf{G} + \mathbf{k}|^2 \delta_{\mathbf{G},\mathbf{G}'} + V. \quad (14)$$

Next, concentrate on the potential term for which we insert an atomistic form that is situated at each atomic site r_a :

$$V_c = \sum_{r_a} V_a(r + r_a) \quad (15)$$

$$V = \frac{1}{\Omega} \int e^{-i(G'+k).r} \sum_{r_a} V_a(r-r_a) e^{i(G+k).r} d\tau \quad (16)$$

$$V = \frac{1}{\Omega} \sum_{r_a} \int V_a(r-r_a) e^{i(G-G').r} d\tau \quad (17)$$

$$r \rightarrow r+r_a \quad V = \frac{1}{\Omega} \sum_{r_a} \int V_a(r) e^{i(G-G').r} d\tau. \quad (18)$$

We turn now to the geometrical structure factor, \mathbf{S} .

$$\text{Separate } \sum_{r_a} \text{ into } \sum_R \sum_t \Rightarrow S = \sum_R \sum_t e^{i(G-G').(R+t)}, \quad (19)$$

so that

$$S = \sum_R e^{i(G-G').R} \sum_t e^{i(G-G').t} \quad G-G' = G''; \quad RG'' = 2\pi n \quad (20)$$

$$S = N \sum_t e^{i(G-G').t} \quad (21)$$

$$V = \frac{N}{\Omega} \sum_t e^{i(G-G').t} \int V_a(r) e^{i(G-G'').r} d\tau. \quad (22)$$

The relation $V/\Omega = 1/\Omega_c$ is the primitive cell volume. For a FCC lattice, $\Omega_c = \frac{A_0^3}{4}$; and A_0^3 is lattice constant.

Pseudopotential form factors are expressed as follows:

$$V = e^{-i(G-G').T} \frac{1}{\Omega_c} \int V_a^{cat}(r) e^{-iq.r} d\tau + e^{i(G-G').T} \frac{1}{\Omega_c} \int V_a^{an}(r) e^{-iq.r} d\tau \quad (23)$$

$q=G'-G$

$$V = [V_f^{an}(q) + V_f^{cat}(q)] \cos(G-G').T + i[V_f^{an}(q) - V_f^{cat}(q)] \sin(G-G').T \quad (24)$$

$$V = V_f^S(q) \cos(G-G').T + iV_f^A(q) \sin(G-G').T \quad (25)$$

Here, $\cos(G-G'') \cdot T$ and $\sin(G-G')$ are the Symmetric anti-symmetric structure factors, respectively.

Then the final form of EPM is written

$$H_{G',G} = \frac{\hbar^2}{2m_0} |G+k|^2 \delta_{G,G'} + V_f^S(q) \cos(G-G').T + iV_f^A(q) \sin(G-G').T. \quad (26)$$

The charge densities from EPM are calculated for the sum of the four valence bands:

$$\psi_{n,\vec{k}}(\vec{r}) = \sum_{\vec{G}} a_{n,\vec{k}}(\vec{G}) e^{i(\vec{G}+\vec{k}).\vec{r}} \quad (27)$$

$$\rho(\vec{r}) = \sum_{n,\vec{k}} \psi_{n,\vec{k}}^*(\vec{r}) \psi_{n,\vec{k}}(\vec{r}), \quad (28)$$

where $\psi_{n,\vec{k}}(\vec{r})$ is the wave function of the valence electron with the wave vector \mathbf{k} in the n^{th} valence band. The summations are taken over the occupied states [16].

3. Results and Discussion

The EPM method is used in the calculation of the zinc-blende GaN and AlN band structures. The experimental measured and calculated energy gap of zinc-blende GaN and AlN using the EPM method are listed in Table 1. We adjust the symmetric and antisymmetric pseudo-potential form factors by fitting the band energies of AlN and GaN obtained by Rubio et al. [17] quasiparticle calculation. The lattice constants a of GaN and AlN used in our calculation are 4.48 and 4.34 Å, respectively. The final adjusted symmetric and antisymmetric form factors of GaN and AlN are shown in Table 2. The band structures of GaN and AlN are shown in Figures 1 and 2, respectively. The results show that GaN is a direct-gap semiconductor with the minimum of conduction band at Γ point, and AlN has an indirect gap with the minimum of conduction band at X point. The calculated energy gaps of GaN E_g^Γ and AlN E_g^X are 3.38 and 5.10 eV, respectively, which are in good agreement with the experimental results. The charge densities from EPM are calculated for the sum of the four valence bands are shown in Figures 3 and 4.

Table 1. The calculated and experimental energy gap for the binary compounds AlN and GaN [18, 19].

	AlN		GAN		
	Calculated	Experimental	Calculated	Experimental	
$E_{\Gamma\Gamma}$ (eV)	5.94	6.0 [18]	3.38	3.1 [18]	3.2 [19]
$E_{\Gamma X}$ (eV)	5.1	4.9 [18]	4.57	4.7 [19]	
$E_{\Gamma L}$ (eV)	9.42	9.3 [18]	5.64	6.2 [19]	

Table 2. Symmetric and antisymmetric form factors and lattice constants of zinc-blende AlN and GaN [18].

$G ^2(2\pi/a)^2 \diamond$	3	4	8	11
V_{AlN}^s	-0.300 [18]		0.080 [18]	0.110 [18]
V_{AlN}^a	0.280 [18]	0.330 [18]		0.015 [18]
V_{GaN}^s	-0.300 [18]		0.060 [18]	0.070 [18]
V_{GaN}^a	0.280 [18]	0.200 [18]		0.040 [18]

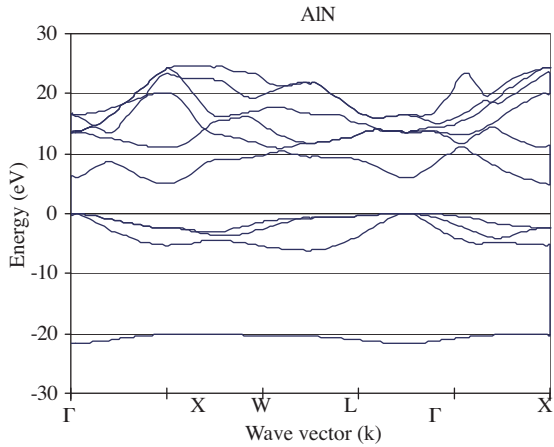


Figure 1. The band structure of zinc-blende AlN.

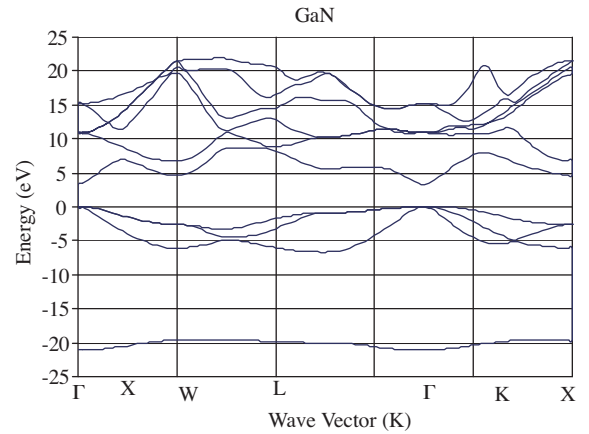


Figure 2. The band structure of zinc-blende GaN.

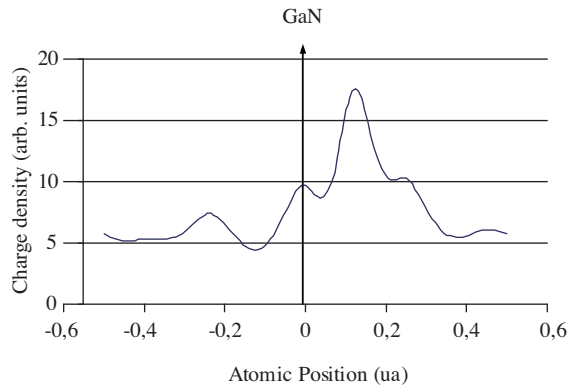


Figure 3. The charge density of zinc-blende GaN.

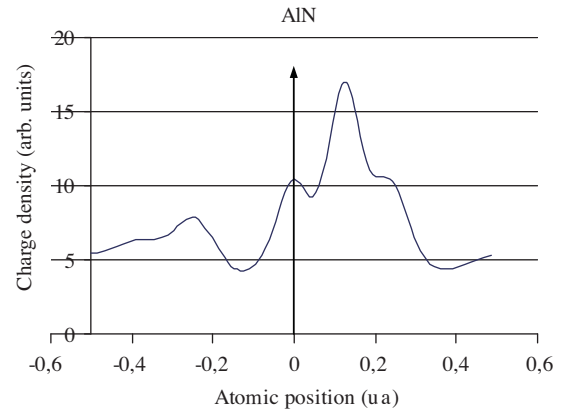


Figure 4. The charge density of zinc-blende AlN.

4. Conclusion

The electronic band structure and the charge density of zinc-blende AlN, GaN, are calculated using an empirical pseudopotential method. It is shown that GaN is a direct-gap semiconductor, with energy gap 3.38 eV. AlN has an indirect, with energy gap 5.10 eV. The charge densities are calculated for the sum of the four valence bands.

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