

CALCULATION OF THE ELECTRON ENERGY STRUCTURE IN AlN, GaN, AND InN CRYSTALS IN THE MIXED BASIS OF SINGLE-PARTICLE STATES

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Electron energy bands in crystalline AlN, GaN, and InN have been calculated in the framework of the density functional theory and making use of a mixed basis. In particular, to calculate the Hamiltonian matrix, the wave functions corresponding to the Bloch states of core electrons together with the plane waves were used. The obtained band structure is in better agreement with experiment than that calculated by the method of *a priori* atomic pseudopotentials in the framework of the local density functional theory.

1. Introduction

Such semiconductors of the A₃B₅-group as AlN, GaN, and InN – as well as their alloys – are new materials intended for applications in high-frequency optoelectronics and for creation of high-power devices [1]. The energy gap widths in those crystals and the alloys on their basis are characterized by values within the range from 1.9 to 6.2 eV. Although modern spectroscopic methods have been applied since the 1980s to study these semiconducting crystals, the parameters of their electron energy bands (interband gaps, effective masses) still remain open for discussion.

This uncertainty disturbs researchers very much, because InN-based heterostructures are very promising for manufacturing lasers, photodiodes, and other devices. Experimental values of the energy gap width E_g at point Γ fall within the interval from 0.7 to 2 eV [2]. At the same time, theoretical values of this parameter do not go beyond the interval from –0.44 to 1.49 eV [3,4].

This work aimed at the *a priori*, i.e. making no use of experimental data, calculation of the electron energy structure in crystalline AlN, GaN, and InN in the mixed basis consisting of the core Bloch functions and the plane waves [5,6].

2. Hamiltonian matrix in the mixed basis and the results of calculation of the electron energy spectrum

The electron energy spectrum of the crystal is sought as a solution of the Schrödinger equation

$$(T + V(\mathbf{r}))\Psi_{\mathbf{k}\alpha}(\mathbf{r}) = E_{\mathbf{k}\alpha}\Psi_{\mathbf{k}\alpha}(\mathbf{r}), \quad (1)$$

where $T = -\nabla^2/2$ is the operator of kinetic energy, V is the potential of an electron in the crystal, and $\Psi_{\mathbf{k}\alpha}$ and $E_{\mathbf{k}\alpha}$ are the wave function and the energy, respectively, of an electron with the wave vector \mathbf{k} in the Brillouin zone and belonging to the α -th energy band. The wave function of an electron in the crystal is sought in the mixed basis as a series

$$\Psi_{\mathbf{k}\alpha}(\mathbf{r}) = \sum_t \sum_{\mathbf{a}} a_{\mathbf{k}t\mathbf{a},\alpha} |\mathbf{k}t\mathbf{a}\rangle + \sum_{\mathbf{G}} a_{\alpha}(\mathbf{k} + \mathbf{G}) |\mathbf{k} + \mathbf{G}\rangle, \quad (2)$$

where $a_{\mathbf{k}t\mathbf{a},\alpha}$ and a_{α} are the variational coefficients of the expansion in core Bloch states

$$|\mathbf{k}t\mathbf{a}\rangle = N^{-1/2} \sum_{\mathbf{A}} e^{i\mathbf{k}(\mathbf{a}+\mathbf{A})} \varphi_t(\mathbf{r} - \mathbf{a} - \mathbf{A}) \quad (3)$$

and plane waves

$$|\mathbf{k} + \mathbf{G}\rangle = \Omega^{-1/2} \exp(i(\mathbf{k} + \mathbf{G})\mathbf{r}). \quad (4)$$

respectively. Here, φ_t are the wave functions of core electrons in the atom [7], the notation $t = \{nlm\}$ means the quantum numbers of those core states, \mathbf{a} stands for the coordinates of the atom in an elementary cell, \mathbf{G} is the reciprocal lattice vector, N is the number of elementary cells in the crystal, \mathbf{A} 's are the Bravais lattice vectors, and Ω is the crystal volume.

By substituting Eq. (2) into Eq. (1), we obtain a system of linear equations in the block form [5, 8]

$$\begin{pmatrix} H_{\mathbf{k}t\mathbf{a},\mathbf{k}'\mathbf{a}'} - ES_{\mathbf{k}t\mathbf{a},\mathbf{k}'\mathbf{a}'} & H_{\mathbf{k}t\mathbf{a},\mathbf{k}+\mathbf{G}'} - ES_{\mathbf{k}t\mathbf{a},\mathbf{k}+\mathbf{G}'} \\ H_{\mathbf{k}+\mathbf{G},\mathbf{k}'\mathbf{a}'} - ES_{\mathbf{k}+\mathbf{G},\mathbf{k}'\mathbf{a}'} & H_{\mathbf{k}+\mathbf{G},\mathbf{k}+\mathbf{G}'} - E\delta_{\mathbf{G},\mathbf{G}'} \end{pmatrix} \times \\ \times \begin{pmatrix} a_{\mathbf{k}t\mathbf{a},\alpha} \\ a_{\alpha}(\mathbf{k} + \mathbf{G}) \end{pmatrix} = 0, \quad (5)$$

where \mathbf{H} is the Hamiltonian matrix, and \mathbf{S} is the overlap matrix in the mixed basis. The upper left block of the matrix in Eq. (5) is calculated using the Bloch functions for core electrons in the atom (B–B), the lower right one using the plane waves (PW–PW), and the upper right one using the mixed functions (the Bloch functions and the plane waves, B–PW). While calculating the matrix elements in system (5), the Cartesian Gaussians [7]

$$\varphi_{nem}(\mathbf{r} - \mathbf{A}) = \sum_i c_i N_i (x - A_x)^l (y - A_y)^m \times \\ \times (z - A_z)^n \exp(-\alpha_i(\mathbf{r} - \mathbf{A})^2) \quad (6)$$

were used, whose parameters c_i and α_i were calculated in the Hartree–Fock approximation; and $N_i = N(\alpha_i)$ are normalization constants. Making use of those Gaussians, the elements of the overlap, \mathbf{S} , and kinetic-energy, \mathbf{T} , matrices in the system of equations (5) can be expressed in the analytical form [9].

Let us calculate the matrix elements for the crystal potential V . The potential of an electron in the crystal is presented as a superposition of contributions made by every lattice site:

$$V(\mathbf{r}) = \sum_{\mathbf{C}} \sum_{\mu} v_{\mu}(\mathbf{r} - \mathbf{c}_{\mu} - \mathbf{C}), \quad (7)$$

where $\mu = \{M, N\}$, $M = \{\text{Al}, \text{Ga}, \text{In}\}$; and $\mathbf{c}_{\mu} = \mathbf{0}$ for $\mu = M$, or $\mathbf{c}_{\mu} = (\mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3)/4$, i.e. a quarter of the cube's diagonal, for $\mu = N$. Every atomic potential v is a sum

$$v(\mathbf{r}) = v_n(\mathbf{r}) + v_e(\mathbf{r}) + v_{xc}(\mathbf{r}) \quad (8)$$

of the nuclear attractive potential v_n , the potential of electron repulsion v_e , and the exchange-correlation potential v_{xc} parameterized in [10].

To speed up calculations, we approximated the dependence $v(\mathbf{r})$ (Eq. (8)) by the formula

$$v(r) = \sum_{i=1}^{n_0} c_i e^{-\beta_i r^2} + \sum_{i=n_0+1}^{n_0+n_2} c_i r^2 e^{-\beta_i r^2} - \\ - Z_n e^{-\lambda r^2} \frac{\text{erf}(\sqrt{p}r)}{r}, \quad (9)$$

where the first two summands are Gaussians, and the third summand simulates the Coulombic component. In expression (9), c_i , β_i , and λ are variational parameters of approximation; Z_n is the number of nuclear protons; and the parameter p determines the depth of the model Coulombic potential well (criteria for its choice have been analyzed by us in [5]). For nitrogen and indium, we put $p = 10^6$. The increase of the p -value gave rise to a deepening of the potential well and a variation of the band energy values by about 0.01 eV.

The elements of potential matrix calculated making use of the first and the second summand in function (9) are analytical expressions [9, 11]. The third summand is more complicated, and we would like to expose here an algorithm for calculations, where this summand is engaged. To take advantage of using the Gaussians in the calculation of three-center integrals, we first carry out the integral transformation

$$\frac{\text{erf}(\sqrt{p}|\mathbf{r}|)}{|\mathbf{r}|} = \frac{2}{\sqrt{\pi}} \int_0^{\sqrt{p}} e^{-u^2 \mathbf{r}^2} du, \quad (10)$$

after which the matrix element calculated using the wave functions for the localized Bloch states reads

$$\langle \mathbf{k}t\mathbf{a} | \frac{\text{erf}(\sqrt{p}|\mathbf{r}|)e^{-s\mathbf{r}^2}}{|\mathbf{r}|} | \mathbf{k}'t'\mathbf{b} \rangle = \\ = \frac{2}{\sqrt{\pi}} \sum_{\mathbf{B}} \sum_{\mathbf{C}} e^{i\mathbf{k}\mathbf{B}} \exp\left[-\frac{\alpha_i \alpha_j}{s_{ij}} (\mathbf{B} + \mathbf{b} - \mathbf{a})^2\right] \times \\ \times \int_0^{\sqrt{p}} \left\{ \exp\left[-\frac{s_{ij}(\lambda + u^2)}{s_{ij} + \lambda + u^2} (\mathbf{C} + \mathbf{c} - \mathbf{D})^2\right] \times \right. \\ \left. \times \int \left[\exp\left[-(s_{ij} + \lambda + u^2)(\mathbf{r} - \mathbf{E})^2\right] \right] \times \right.$$

$$\begin{aligned} & \times (x - a_x)^{L1} (y - a_y)^{M1} (z - a_z)^{N1} (x - b_x - B_x)^{L2} \times \\ & \times (y - b_y - B_y)^{M2} (z - b_z - B_z)^{N2} \Big] d\mathbf{r} \Big\} du, \end{aligned} \quad (11)$$

where $s_{ij} = \alpha_i + \alpha_j$. When deriving Eq. (11), we applied – twice – the theorem on the product of two Gaussians centered at different sites. The product is equal to a third Gaussian,

$$e^{-\alpha(\mathbf{r}-\mathbf{A})^2} e^{-\beta(\mathbf{r}-\mathbf{B})^2} = e^{-\frac{\alpha\beta}{\alpha+\beta}(\mathbf{B}-\mathbf{A})^2} e^{-(\alpha+\beta)(\mathbf{r}-\mathbf{D})^2} \quad (12)$$

centered at the site

$$\mathbf{D} = \frac{\alpha\mathbf{A} + \beta\mathbf{B}}{\alpha + \beta}. \quad (13)$$

The first application of formulas (12) and (13) gives rise to the following coordinates of a new center:

$$\mathbf{D} = \frac{\alpha_i \mathbf{a} + \alpha_j (\mathbf{b} + \mathbf{B})}{s_{ij}}. \quad (14)$$

The next application of those formulas results in a new center of Gaussian localization in formula (11):

$$\mathbf{E} = \frac{s_{ij} \mathbf{D} + (\lambda + u^2)(\mathbf{c} + \mathbf{C})}{s_{ij} + \lambda + u^2}. \quad (15)$$

The integration in Eq. (11) is carried separately over each coordinate. However, all expressions must be first reduced to a single common center by substituting the coefficient in the exponent according to the formula $s = s_{ij} + \beta + u^2$:

$$\begin{aligned} & \int (x - a_x)^{L1} (x - b_x - B_x)^{L2} e^{-(s_{ij} + \beta + u^2)(x - \mathbf{E}_x)^2} dx = \\ & = \int ((x - E_x) + (E_x - a_x))^{L1} \times \\ & \times ((x - E_x) + (E_x - b_x - B_x))^{L2} e^{-s(x - \mathbf{E}_x)^2}. \end{aligned} \quad (16)$$

Then, we expand the Newton binomials on the right-hand side of Eq. (16) and write down it in the following form:

$$\begin{aligned} & \sum_{ix=0}^{L1} \sum_{jx=0}^{L2} \binom{ix}{L1} \binom{jx}{L2} \times \\ & \times (E_x - a_x)^{L1-ix} (E_x - b_x - B_x)^{L2-jx} I_x(ix + jx, s), \end{aligned} \quad (17)$$

where

$$\begin{aligned} I_x(n) &= \int (x - E_x)^n e^{-s(x - \mathbf{E}_x)^2} dx = \\ &= \begin{cases} (n-1)\sqrt{\pi}2^{-n/2}s^{-(n+1)/2}, & n - \text{even}, \\ 0, & n - \text{odd}. \end{cases} \end{aligned} \quad (17a)$$

At last, on the basis of Eqs. (11)–(17), we obtain the calculation formula for the element of the potential energy matrix (the third summand on the right-hand side of Eq. (9)):

$$\begin{aligned} & \frac{2}{\sqrt{\pi}} \sum_{\mathbf{B}} e^{i\mathbf{k}\mathbf{B}} \exp\left[-\frac{\alpha_i \alpha_j}{s_{ij}} (\mathbf{B} + \mathbf{b} - \mathbf{a})^2\right] \times \\ & \times \sum_{\mathbf{C}} \int_0^{\sqrt{p}} \exp\left[-\frac{s_{ij}(\beta + u^2)}{s_{ij} + \beta + u^2} (\mathbf{C} + \mathbf{c} - \mathbf{D})^2\right] \times \\ & \times \left[\sum_{ix=0}^{L1} \sum_{jx=0}^{L2} \binom{ix}{L1} \binom{jx}{L2} (E_x - a_x)^{L1-ix} \times \right. \\ & \times (E_x - b_x - B_x)^{L2-jx} I_x(ix + jx, s) \times \\ & \times \sum_{iy=0}^{M1} \sum_{jy=0}^{M2} \binom{iy}{M1} \binom{jy}{M2} (E_y - a_y)^{M1-iy} \times \\ & \times (E_y - b_y - B_y)^{M2-jy} I_y(iy + jy, s) \times \\ & \times \sum_{iz=0}^{N1} \sum_{jz=0}^{N2} \binom{iz}{N1} \binom{jz}{N2} (E_z - a_z)^{N1-iz} \times \\ & \left. \times (E_z - b_z - B_z)^{N2-jz} I_z(iz + jz, s) \right] du. \end{aligned} \quad (18)$$

The one-dimensional integration in expression (18) was executed with the help of the Gauss quadrature formula [12]. The number of integration nodes was selected so that a further increase of their number would not give rise to the variation of band energy values by more than 10^{-4} eV.

Now, the elements in the matrices associated with overlapping, kinetic energy, and first two components of the crystal potential (9) in the system of equations (5) are analytical expressions in all their blocks. The calculation of coefficients in Eq. (5) was completed by carrying out the numerical integration in Eq. (18). The solution of system (5) gives us the required energy of electrons in the crystal.

The results of calculations of the electron energy spectrum in the crystals concerned are summarized in Tables 1 to 3, the titles of which also indicate the

number of equations N included in system (5). For instance, in the case of AlN, 875 equations ($N = 875$) were used to determine 5 core Bloch states of aluminum ($1s$, $2s$, $2p_x$, $2p_y$, and $2p_z$), 1 core Bloch state of nitrogen ($1s$), and 869 plane waves. The last sphere in the momentum space totally filled by the latter corresponded to the sum of squared Miller indices $h^2 + k^2 + l^2 = 88$. A further increase of the plane wave number in Eq. (2) did not result in noticeable variations of the band energies; and that is why we confined ourselves to N -values quoted here in the case of the crystals concerned. Columns MB in the Tables contain our results, which were calculated for the system of equations (5) in the framework of the mixed basis method. Columns LDA- d and LDA+ d contain the results of calculations of the electron band energies [2] by the *a priori* method of atomic pseudopotentials without and with the inclusion of Ga's $3d$ -states and In's $4d$ -ones into the basis, respectively.

Column EXX in Table 1 includes the results of calculations of band energies by the method of exact exchange potential [3,4]. Columns EXX- d and EXX+ d in Tables 2 and 3 contain the results of calculations by the method of exact exchange potential without and with the inclusion of Ga's $3d$ -states and In's $4d$ -ones into the basis, respectively. Experimental data were taken from work [4]. Striking is a small number of experimental data for the band energy values in all three crystals concerned.

The results of calculations were obtained by other authors in the local density approximation (LDA), making use of the electron exchange-correlation potential and the formulas which are accurate in the

Table 1. Electron energy values (in eV) at points Γ , X , and L of the first Brillouin zone in an AlN crystal, $N = 875$

Level	MB	LDA	EXX	Exp.
Γ_{1v}	-15.30			
Γ_{15v}	0.00	0.00	0.00	0.00
Γ_{1c}	5.01	4.27	5.74	
Γ_{15c}	13.81			
X_{3v}	-4.26			
X_{5v}	-1.52			
X_{1c}	5.30	3.27	5.06	5.11
X_{1c}	9.95			
X_{3c}	15.04			
L_{1v}	-13.72			
L_{1v}	-4.99			
L_{3v}	-0.42			
L_{1c}	8.40	7.25	8.58	
L_{1c}	11.39			
L_{3c}	12.70			

limit of a uniform electron density distribution [10]. In the LDA- d approximation, the wave functions of $3d$ - or $4d$ -electrons are associated with the core states of atoms. On the contrary, the LDA+ d one supposes that the Bloch functions of those electrons are included into the basis along with plane waves (2).

The EXX- d and EXX+ d approximations are based on knowing the exact exchange potential for all atomic electrons at the stage of parameter calculations for the *a priori* pseudopotentials and only for valence electrons at a stage of band energy calculations (see Tables 1 to 3).

For level Γ_{1c} , a decrease of its energy value, i.e. a deterioration of the result, is observed at the transition from the LDA- d approximation to the LDA+ d one, and an increase, i.e. an improvement, of the result on changing from the EXX- d to the EXX+ d approximation. This tendency is repeated for the lower level X_{1c} , but is opposite for the even lower level L_{1c} .

The EXX approximation is much more accurate as compared with the LDA, although the computational algorithms engaged in the EXX approximation are slower. The data presented in Table 3 demonstrate that the LDA can hardly be applicable to crystals with narrow interband gaps.

Tables 2 and 3 also demonstrate that the energy values obtained for the bottom of the valence band in the LDA are, as a rule, lower than those obtained in the MB and EXX approximations. The case LDA+ d (Table 3) is an exception, where the bottom of the valence band lies lower than that in the EXX- d case; however, the corresponding width of the energy gap turns out negative, which contradicts the experiment.

Table 2. Electron energy values (in eV) at points Γ , X , and L of the first Brillouin zone in an GaN crystal, $N = 1082$

Level	MB	LDA- d	LDA+ d	EXX- d	EXX+ d	Exp.
Γ_{1v}	-16.47	-15.5	-16.3	-16.7	-17.8	
Γ_{15v}	0.00	0.00	0.00	0.00	0.00	0.00
Γ_{1c}	2.49	2.0	1.9	2.8	3.1	3.2
Γ_{15c}	11.52	10.2	10.6	11.3	12.2	
X_{1v}	-15.30	-12.4	-13.0	-13.5	-14.8	
X_{3v}	-5.29	-6.1	-6.5	-6.8	-6.9	
X_{5v}	-2.66	-2.4	-2.8	-2.7	-3.0	
X_{1c}	4.92	3.3	3.2	4.4	4.7	
X_{1c}	8.11	6.6	6.9	7.7	8.4	
X_{3c}	12.45	11.9	12.2	14.0	14.5	
L_{1v}	-15.51	-13.2	-13.8	-14.3	-15.5	
L_{1v}	-6.53	-6.8	-7.0	-7.6	-7.5	
L_{3v}	-0.95	-0.8	-1.0	-0.9	-1.1	
L_{1c}	5.82	4.8	4.7	6.1	5.7	
L_{1c}	9.73	8.9	9.1	10.4	11.2	
L_{3c}	11.65	10.3	10.6	11.3	12.3	

3. Conclusions

Making use of no experimental data, the characteristic energies of electrons in AlN, GaN, and InN crystals have been calculated in the framework of the mixed basis method. Formally, the MB method is related to the LDA one; however, the latter is based only on *a priori* atomic pseudopotentials and on the plane-wave basis. Table 3 demonstrates a contradiction between the energy values for the bottom of the conduction band obtained in the LDA. Really, the energy value obtained for level Γ_{1c} by the more consistent LDA+d method is negative and, as such, has no physical meaning, although, from logical reasoning, it should have been better than that found in the framework of the LDA-d approach.

The values of band energies obtained taking into account the interactions between core and valence electrons in the LDA are close to the corresponding results found in the framework of the exact exchange potential method. Hence, taking into consideration the hybrid block structure of the overlap matrix and the Hamiltonian in the system of equations (5) improves the quality of the band energy calculation results to the level which is characteristic of the more complicated but more consistent EXX method. Using the MB method, the considerably better values for electron band energies can be obtained even in the LDA. This circumstance follows from a basic difference between the LDA-based MB and pseudopotential approaches: in the MB method, the fact that an atom in the crystal is surrounded by other atoms of the same or other kinds is consistently

taken into account in all blocks of the system of equations (5), while the pseudopotential parameters are “frozen” at a level of atomic data and are not changed under the action of the crystalline environment. The verification of this assumption making use of others crystals will be the purpose of our further researches.

Table 3. Electron energy values (in eV) at points Γ , X , and L of the first Brillouin zone in an InN crystal, $N = 965$

Level	MB	LDA-d	LDA+d	EXX-d	EXX+d	Exp.
Γ_{1v}	-15.02	-13.99	-14.60	-14.37	-14.74	
Γ_{15v}	0.00	0.00	0.00	0.00	0.00	0.00
Γ_{1c}	1.23	0.27	-0.44	1.49	0.81	0.7, 1.0, 1.9
Γ_{15c}	10.80					
X_{1v}	-13.21					
X_{3v}	-4.08					
X_{5v}	-1.81					
X_{1c}	4.66	2.87	2.82	4.63	4.20	
X_{1c}	7.96					
X_{3c}	10.60					
L_{1v}	-4.73					
L_{3v}	-0.62					
L_{1c}	4.84	3.51	2.95	4.75	4.14	
L_{1c}	8.36					
L_{3c}	10.82					

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ЕЛЕКТРОННА ЕНЕРГЕТИЧНА СТРУКТУРА КРИСТАЛІВ AlN, GaN та InN, РОЗРАХОВАНА В ЗМІШАНОМУ БАЗИСІ ОДНОЧАСТИНКОВИХ СТАНІВ

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Резюме

Розраховано електронні енергетичні спектри кристалів AlN, GaN та InN у змішаному базисі у наближенні функціонала локальної електронної густини. Матрицю гамільтоніана обчислено на функціях Блоха глибоких електронів та плоских хвилях. Отримані зонні енергії краще узгоджуються з експериментом, ніж розраховані методом атомних апріорних псевдопотенціалів у наближенні функціонала локальної електронної густини.