Semiempirical tight-binding modelling of III-N-based heterostructures

H. Hakan Gürel, Özden Akinci, Hilmi Ünlü

Abstract

In this work, we present a second nearest neighbour sp³s* semi-empirical tight-binding theory to calculate the electronic band structure of heterostructures based on group III-N binary semiconductors and their ternaries. The model Hamiltonian includes the second nearest neighbour (2nn) interactions, the spin–orbit splitting and the nonlinear variations of the atomic energy levels and the bond length with ternary mole fraction. Using this sp³s* tight-binding approach, we investigated the electronic band structure of Al₁₋ₓGaₓN/GaN and In₁₋ₓGaₓN/GaN heterostructures as a function of composition and interface strain for the entire composition range (0 ≤ x ≤ 1). There is an excellent agreement between the model predictions and experiment for the principal bandgaps at Γ, L and X symmetry points of the Brillouin zone for AlN, GaN and InN binaries and Al₁₋ₓGaₓN and In₁₋ₓGaₓN ternaries. The model predicts that the composition effects on the valence band offsets is linear, but on the conduction band offsets is nonlinear and large when the interface strain and deformation potential is large.

Keywords: Tight-binding theory; Heterostructures; Bandgaps; Band offsets; Nitrides

1. Introduction

The epitaxial growth of novel semiconductor heterostructures based on III-nitride compounds (e.g. superlattices, quantum wells, or quantum dots) has become vital in the production of high-performance electronic and optoelectronic devices in recent years [1,2]. Advanced growth
techniques, such as molecular beam epitaxy and the metalorganic vapour-phase epitaxy makes it now possible to control and tailor the material properties of almost any ternary semiconductor during growth. For example, indirect and direct bandgap binaries can form ternary alloys with a direct fundamental bandgap over the entire composition range. Group III-nitride compounds (GaN, AlN, InN) and their ternary alloys (AlGaN, InGaN, InAlN) have been the subject of intense work in recent years due to the possibility of achieving blue or ultraviolet light-emitting and laser diodes, blue resonant-cavity light-emitting diodes and surface-emitting lasers, and solar blind ultraviolet photodetectors, as well as high-power high-frequency field-effect transistors. However, it is well known that there is a considerable lattice mismatch strain across the interface in heterostructures made from group III-nitrides and their ternary alloys. For example, large strain builds up in the GaN/AlN heterostructures because the lattice mismatch is of the order of 2.4%, raising the question of strain relaxation even for thin epitaxial GaN or AlN layers. The optical properties of GaN/AlGaN quantum wells or GaN/AlN quantum dots are modified by strain induced piezoelectric polarization. Therefore, quantitatively accurate and qualitatively reliable modelling of the electronic structure of these materials as a function of strain, temperature and alloy composition allows better controlling of their material properties during the growth in utilizing them for high performance electronic and optical device applications.

There are two theoretical methods for calculating the electronic band structure of semiconductors and their heterostructures; the empirical pseudopotential method [4] and semi-empirical tight-binding method [5–11]. The pseudopotential model calculations of electronic band structures are computationally intensive and cannot be easily implemented for the study of some practical electronic and optical devices at nano dimensions. Meanwhile, the tight-binding model calculations of electronic band structures are known to be simpler, but reliable and relatively easier to implement in calculating the electronic properties of heterostructures with low dimensions [3]. In this work, we have developed an accurate and reliable semi-empirical sp$^3$s$^*$ tight-binding model to calculate the electronic band structure of semiconductor heterostructures based on group III-nitrides and ternary alloys. The model Hamiltonian fully accounts for the observed experimental data and reproduces the empirical pseudopotential calculations of principal bandgaps at high symmetry points in the Brillouin zone of bulk AlN, GaN and InN and Al$_{1-x}$Ga$_x$N and In$_{1-x}$Ga$_x$N ternaries with cubic crystal structure. The sp$^3$s$^*$ tight-binding Hamiltonian includes the second nearest neighbour (2nn) interaction of the atoms and spin–orbit coupling. Adding the s$^*$ excited state with spin–orbit coupling to the sp$^3$ parametrization makes it possible to accurately calculate the conduction band structure features at the $\Gamma$ and X high symmetry points. The inclusion of the second nearest neighbour interactions in the sp$^3$s$^*$ tight binding model yields better fit of the conduction band at the L symmetry point. In Section 2, we give a brief review of the semi-empirical sp$^3$s$^*$ tight-binding theory to study the composition effects on the group II–VI ternary alloy semiconductors. In Section 3, we discuss our results about the composition and strain effects on bandgaps and band offsets in AlGaN/GaN and InGaN/GaN heterostructures.

2. Tight-binding method of band structure calculations

The semi-empirical sp$^3$s$^*$ tight-binding approach allows the precise and reliable modelling of effects of shape, size, and atomic scale variation in alloy composition on the electronic states in the low dimensional heterostructures [3]. The sp$^3$s$^*$ tight-binding Hamiltonian is easily obtained by adjusting the diagonal and off-diagonal (hopping) matrix elements to reproduce the known bandgaps of bulk semiconductors by using the least-squared error minimization fitting procedure.
at a number of high symmetry points in the band dispersion curves to fit the band dispersion curve obtained from the empirical pseudopotential method [4]. We have adopted the well-known semi-empirical \(sp^3s^*\) tight-binding theory [8,9] of semiconductors in order to obtain a qualitatively realistic and quantitatively precise tight-binding model, with accurate parameters, for group III-nitride compounds AlN, GaN and InN and their ternary alloys AlGaN, InGaN and InAlN with cubic structure. In this \(sp^3s^*\) tight-binding model each cation atom (Ga, Al, and In) and anion atom (N) are described by their outer valence s orbital, the three outer p orbitals and a fictitious excited s* orbital added to mimic the effects of higher lying states. The spin–orbit effects are included by coupling different spin states of different on-site p orbitals through the spin–orbit interaction. In the \(sp^3s^*\) tight-binding context Schrodinger equation is written as:

\[
\sum_{\beta} \left[ H_{\alpha\beta}(k) - S_{\alpha\beta}(k) E \right] \mu_{\beta} = 0 \tag{1}
\]

where \(E\) is the energy eigenvalue of the \(10 \times 10\) Hamiltonian matrix \(H_{\alpha\beta} = \langle \chi_{\alpha}(k) | H | \chi_{\beta}(k) \rangle\) and \(S_{\alpha\beta} = \langle \chi_{\alpha}(k) | \chi_{\beta}(k) \rangle\) is the overlap integral between the atomic-like orbitals, with \(\alpha\) and \(\beta\) that correspond to a cation (c) and anion (a) s (p) orbitals, respectively. \(\chi(k)\) is the basis function formed by the linear combination of cation and anion s (p) atomic orbitals and \(\mu_{\beta}\) is the wave function coefficient. The \(sp^3s^*\) tight-binding Hamiltonian matrix \(H_{\alpha\beta}\), has thirteen independent matrix elements; six diagonal elements (on-site atomic energies), \(E_{sa}, E_{sc}, E_{pa}, E_{pc}, E_{s^*a}\) and \(E_{s^*c}\), on the cation (Al, Ga and In) and anion (N) atoms, and the seven off-diagonal elements (transfer matrix elements) known as hopping terms, \(E_{ss}, E_{sx}, E_{sa}, E_{pa}, E_{pc}, E_{s^*a}\) and \(E_{s^*c}\) and finally two second-nearest neighbour transfer matrix elements, \(\epsilon_{sx}\) and \(\epsilon_{xy}\). Here s and p refers to the basis states and a and c refer to anion (N) and cation (Al, Ga and In) atoms. The inclusion of 2nn interactions in the \(sp^3s^*\) tight-binding Hamiltonian introduces two additional interaction parameters, \(\epsilon_{sx}\) and \(\epsilon_{xy}\) [13]. The inclusion of the spin–orbit coupling in the \(sp^3s^*\) tight binding model increases the size of the \(10 \times 10\) Hamiltonian matrix to a \(20 \times 20\) one that is diagonalized for each \(k\) vector to obtain the semiconductor electronic band structure [3].

The \(sp^3s^*\) tight-binding parameters introduced above are determined and optimized by focusing on the reproduction of the bandgap energies at high symmetry points in the energy dispersion curve obtained from the pseudopotential approach [4] as verified by the experiment [12]. These optimized \(sp^3s^*\) tight-binding parameters are then used for calculations of the electronic structure of Al\(_{1-x}\)Ga\(_x\)N/GaN and In\(_{1-x}\)Ga\(_x\)N/GaN ternary/binary III-nitride semiconductor heterostructures. Table 1 gives the list of the optimized 1nn and 2nn \(sp^3s^*\) tight-binding parameters obtained from reproducing the energy bands in the energy dispersion curve of AlN, GaN and InN bulk III-nitrides due to pseudopotential theory [4] and experiment [12]. In this table, the tight-binding interaction parameters \(4V_{sp^*}\) and \(4V_{ps^*}\) were adjusted to fit to the X bandgaps and the 2nn interaction parameters \(\epsilon_{sx}\) and \(\epsilon_{xy}\) to get a good fit to the L bandgaps in reproducing the pseudopotential energy bands in the energy dispersion curve [4]. Fig. 1a–c displays the results of our calculations for AlN, GaN and InN bulk III-nitrides. One can see from Fig. 1a–c, the inclusion of the excited s*–state to the \(sp^3\) basis set on the cation (Al, Ga and In) and anion (N) atoms, with the second nearest neighbour interactions and the spin–orbit coupling, makes it possible to simulate better the conduction bands of III-nitride semiconductors, which cannot be done with the \(sp^3\) tight binding model [5–7].

3. III-N ternary/binary heterostructure modelling

The main advantage of ternary alloy semiconductors is that their principal energy gaps and lattice parameters can be tailored independently to fabricate devices on suitable lattice
Table 1

Tight-binding parameters for AlN, GaN and InN compounds obtained from the fitting of 2nn the sp\textsuperscript{3}s* tight-binding model bands to the pseudopotential bands \cite{4} and measured bandgaps \cite{17} at high symmetry points

<table>
<thead>
<tr>
<th></th>
<th>AlN</th>
<th>GaN</th>
<th>InN</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_{s,a}$</td>
<td>$-11.5047$</td>
<td>$-12.9156$</td>
<td>$-12.8605$</td>
</tr>
<tr>
<td>$E_{p,a}$</td>
<td>$4.3815$</td>
<td>$3.1697$</td>
<td>$1.9800$</td>
</tr>
<tr>
<td>$E_{s,c}$</td>
<td>$0.5047$</td>
<td>$-1.5844$</td>
<td>$-0.3994$</td>
</tr>
<tr>
<td>$E_{p,c}$</td>
<td>$10.2184$</td>
<td>$9.0302$</td>
<td>$8.0200$</td>
</tr>
<tr>
<td>$E_{s,a}^*$</td>
<td>$12.0400$</td>
<td>$12.2000$</td>
<td>$10.6300$</td>
</tr>
<tr>
<td>$E_{s,c}^*$</td>
<td>$13.7400$</td>
<td>$13.0000$</td>
<td>$10.0000$</td>
</tr>
<tr>
<td>$4V_{s,s}$</td>
<td>$-9.8077$</td>
<td>$-8.8996$</td>
<td>$-4.2285$</td>
</tr>
<tr>
<td>$4V_{x,x}$</td>
<td>$6.6900$</td>
<td>$5.3500$</td>
<td>$3.9800$</td>
</tr>
<tr>
<td>$4V_{x,y}$</td>
<td>$8.9400$</td>
<td>$8.6200$</td>
<td>$7.4100$</td>
</tr>
<tr>
<td>$4V_{a,pc}$</td>
<td>$7.8500$</td>
<td>$6.4000$</td>
<td>$3.8100$</td>
</tr>
<tr>
<td>$4V_{pa,sc}$</td>
<td>$7.6800$</td>
<td>$7.2400$</td>
<td>$6.1900$</td>
</tr>
<tr>
<td>$4V_{s,a,pc}$</td>
<td>$8.0300$</td>
<td>$7.0600$</td>
<td>$6.8800$</td>
</tr>
<tr>
<td>$4V_{pa,s,c}$</td>
<td>$2.4700$</td>
<td>$1.8200$</td>
<td>$3.3600$</td>
</tr>
<tr>
<td>(\varepsilon_{s,x})</td>
<td>$-1.4000$</td>
<td>$0.9500$</td>
<td>$0.6150$</td>
</tr>
<tr>
<td>(\varepsilon_{s,y})</td>
<td>$6.9000$</td>
<td>$0.1000$</td>
<td>$0.7100$</td>
</tr>
<tr>
<td>(\lambda_d)</td>
<td>$0.0035$</td>
<td>$0.0035$</td>
<td>$0.0035$</td>
</tr>
<tr>
<td>(\lambda_c)</td>
<td>$0.0070$</td>
<td>$0.0410$</td>
<td>$0.1100$</td>
</tr>
</tbody>
</table>

The model parameters were taken from Refs. \cite{17,18} but revised and optimized to get better fit to the energy bands obtained by the pseudopotential theory \cite{4}.

matched substrates. Most of the electronic and optical devices based on group III-nitrides consist of ternary/binary combination such as Al\(_{1-x}\)Ga\(_x\)N/GaN and In\(_{1-x}\)Ga\(_x\)N/GaN because their energy gap covers various light spectra over the entire alloy composition. Group III-nitride ternary/binary heterostructures have been the subject of intense work in recent years due to the possibility of achieving blue or ultraviolet light-emitting and laser diodes, blue resonant-cavity light-emitting diodes and surface-emitting lasers, and solar blind ultraviolet photodetectors, as well as high-power high-frequency field-effect transistors. However, there is a considerable lattice mismatch strain across the ternary/binary interface in III-N heterostructures. Therefore, our main goal is to use the 2nn the sp\textsuperscript{3}s* semi-empiric tight-binding theory, discussed in the previous Section 2, to determine the alloy composition and lattice mismatch induced interface strain effects on the band structure of Al\(_{1-x}\)Ga\(_x\)N/GaN and In\(_{1-x}\)Ga\(_x\)N/GaN heterostructures. In the context of second nearest neighbour sp\textsuperscript{3}s* tight-binding theory, we shall first formulate the bond length of ternary semiconductors in which the effect of composition disorder is described appropriately in terms of the host bond length and the distorted bond length by the substitutional impurity without any adjustable parameter \cite{10,11}. The so called virtual crystal approximation (VCA) is commonly used to determine the tight-binding Hamiltonian matrix elements and the bond length of the ternary alloy with and without the compositional disorder. However, detailed treatment requires the inclusion of compositional disorder effect on the structural and electronic properties of ternary alloy \cite{10,11,14}. The composition variation of the A\(_{1-x}\)B\(_x\)C ternary alloy semiconductor is written as sum of undistorted bond length due to virtual crystal approximation (VCA) and the distorted term due to cation–anion relaxation given as: \cite{10,11,14}

\[
d(x) = d_{\text{VCA}} + d_{\text{relax}} = (1 - x)d_{0AC} + xd_{0BC} + x(1 - x)\delta_c(d_{BC}(x) - d_{AC}(x))
\]

where \(d_{0AC}\) and \(d_{0BC}\) are the undistorted bond lengths of host materials AC and BC and \(d_{AC}(x)\), \(d_{BC}(x)\) are the bond lengths of AC and BC binaries in A\(_{1-x}\)B\(_x\)C ternary
Fig. 1. Band structure of AlN, GaN and InN binary semiconductor at 0 K, obtained by using the tight-binding parameters given in Table 1.

\[
d_{\text{BC}}(x) = (1 - x)d_{\text{AC}}^0 + xd_{\text{BC}}^0 + (1 - x)\xi_{\text{BC}:A}(d_{\text{BC}}^0 - d_{\text{AC}}^0)
\]
\[
d_{\text{AC}}(x) = (1 - x)d_{\text{AC}}^0 + xd_{\text{BC}}^0 + x\xi_{\text{AC}:B}(d_{\text{AC}}^0 - d_{\text{BC}}^0)
\]

where \(\xi_{\text{AC}:B}\) and \(\xi_{\text{BC}:A}\) are the dimensionless relaxation parameters [15]. In Eq. (2) \(\delta_c\) is the difference between dimensionless relaxation parameters \(\xi_{\text{AC}:B}\) and \(\xi_{\text{BC}:A}\) [15]

\[
\delta_c = \xi_{\text{AC}:B} - \xi_{\text{BC}:A} = \frac{1}{1 + \frac{\alpha_{\text{AC}}}{\alpha_{\text{BC}}}(1 + 10\frac{\beta_{\text{AC}}}{\beta_{\text{BC}}})} - \frac{1}{1 + \frac{\alpha_{\text{BC}}}{\alpha_{\text{AC}}}(1 + 10\frac{\beta_{\text{BC}}}{\beta_{\text{AC}}})}.
\]

We are now ready in principle to use Eq. (2) to take into account the composition variations of the transfer matrix elements (off-diagonal elements; \(E_{\text{ss}}, E_{\text{sx}}, E_{\text{sp}}, E_{\text{sc}}, E_{\text{xy}}, E_{\text{sp}}, E_{\text{ps}}, E_{\text{ps}}\)) in the sp\(^3\)s\(^*\) tight-binding Hamiltonian matrix, given in Table 1 for \(A_1 - xB_xC\) ternary semiconductor. Likewise, the diagonal matrix elements (on-site atomic energies; \(E_{\text{sa}}, E_{\text{sc}}, E_{\text{pa}}, E_{\text{pc}}, E_{\text{s}^*\text{a}}\) and \(E_{\text{s}^*\text{c}}\)) in the sp\(^3\)s\(^*\) tight-binding Hamiltonian matrix, given in Table 1. The on-site atomic energies (\(E_{\text{sa}}, E_{\text{sc}}, E_{\text{pa}}, E_{\text{pc}}, E_{\text{s}^*\text{a}}\) and \(E_{\text{s}^*\text{c}}\)) and transfer matrix elements (\(E_{\text{sa}}, E_{\text{sx}}, E_{\text{sp}}, E_{\text{sc}}, E_{\text{xy}}, E_{\text{sp}}, E_{\text{ps}}\) and \(E_{\text{ps}}\)) of the sp\(^3\)s\(^*\) tight-binding Hamiltonian matrix for \(A_1 - xB_xC\) ternary semiconductor are assumed to be a nonlinear function of alloy composition: [10,11]

\[
E_{\alpha/\beta}(x) = (1 - x)E_{\alpha/\beta}(\text{AC}) + xE_{\alpha/\beta}(\text{BC}) + x(1 - x)\delta_c \Delta E_{\alpha/\beta}
\]
where $\Delta E_{\alpha/\beta} = E_{\alpha/\beta}(\text{AC}) - E_{\alpha/\beta}(\text{BC})$, with $\alpha$ and $\beta$ representing the fitted energies of the s and p states of the anion (N) and cation (Al, Ga and In) atoms forming the AC and BC compounds. Using the optimized sp$^3$s$^*$ tight binding model parameters for AlN, GaN and InN given in Table 1, we can now accurately calculate the composition effects on the electronic band structure of Al$_{1-x}$Ga$_x$N/GaN and In$_{1-x}$Ga$_x$N/GaN heterostructures.

4. Results and discussion

The demonstration of stimulated emission in the blue spectral region from nitride-based boosted efforts to get better understanding of the electronic and optical properties of ternary/binary III-N heterostructures. Because the advanced growth techniques such as molecular beam epitaxy (MBE) makes it possible to control and tailor the ternary semiconductor bandgaps and lattice parameters so that these materials with different compositions can be grown on a suitable lattice matched substrate. As with all of the semiconductor devices, the key property to understand and appreciate the potential impact of III-N based heterostructures on the performance of photonic devices is the composition and strain variation of their electronic energy band structure across the interface. The conduction and valence band offsets $\Delta E_c$ and $\Delta E_v$ at interface between the constituent semiconductors control the electronic and optical properties of heterostructure devices. Therefore, the reliable and precise modelling of interface energy band structure highly crucial in the design and optimization of III-N semiconductor electronic and photonic devices. We can use the 2nn sp$^3$s$^*$ empirical tight-binding model discussed in the previous sections to investigate the composition and interface strain effects on the bandgaps and band offsets of III-N ternary/binary heterostructures. Specifically, we shall focus on the electronic band structure of Al$_{1-x}$Ga$_x$N/GaN and In$_{1-x}$Ga$_x$N/GaN heterostructures for which there is experimental data available for the principal bandgap energies to compare. Furthermore, these heterostructures are important for photonic applications, but there is a considerable lattice mismatch strain across their interfaces over most of the composition range. The macroscopic observable consequences of interface strain, due to lattice mismatch and/or thermal expansion gradient, are the changes in the structural and electronic properties (e.g. lattice constant, bandgap, band offset, effective mass, etc.) that determines the carrier transport across the heterostructure and then affects the device performance. The effects of interface strain effects on the energy band properties of ternary/binary III-nitrides based heterostructures can be easily determined by integrating the so called statistical thermodynamic model of semiconductors [16] with the 2nn sp$^3$s$^*$ tight- binding model discussed previously. Limiting the discussion on the technologically important (001) strained heteroepitaxy, elastic theory yields the strain in barrier parallel and perpendicular to the interface, equal to that in the well but different in the barrier:

$$\epsilon_{xx} = \epsilon_{yy} = \epsilon_{f \parallel} = \frac{a_f - a}{a_f} a_f \parallel = a_s$$

$$\epsilon_{zz} = -2 \frac{C_{12}}{C_{11}} \epsilon_{xx} = \epsilon_{f \perp} = \frac{a_\perp - a}{a} a_f \perp = a_f - 2 \frac{C_{12}}{C_{11}} \epsilon_{f \parallel}$$

where $a_s$ and $a_f$ are the lattice constants of the substrate and epilayer and $C_{11}$ and $C_{12}$ are elastic constants semiconductors. According to the statistical thermodynamic model of semiconductors [16], one first expresses the conduction and valence band energy levels as a function of hydrostatic pressure at any temperature as:
where $E_{cl}$ and $E_v$ are the conduction minimums and valence band maximum at $\Gamma$, L and X symmetry points with deformation potentials $a_{cl} = -B(\partial E_{cl}/\partial P)$ and $a_v = -B(\partial E_v/\partial P)$, $B$ is the bulk modulus with its derivative $B' = \partial B/\partial P$. The coefficients $C^0_{cP} = C^0_{nP} - C^0_{0P} = C^0_{pP} + \Delta C^0_P$ and $C^0_{vP} = C^0_{pP}$ are the standard heat capacities of conduction electrons and valence holes; $C^0_{nP} = C^0_{pP} = (5/2)k$, where $k$ is the Boltzmann’s constant. $\Delta C^0_P = C^0_{nP} + C^0_{pP} - C^0_{0P}$ is the heat capacity of reaction of free electron and hole formation obtained from fitting the predicted bandgap to experiment. While the uniaxial strain component splits the heavy-hole, light-hole and split-off valence band edges at $\Gamma$ symmetry point, the hydrostatic strain component shifts the position of the conduction and valence band edges relative to the average valence band edge [16]. For (001) crystal growth, $P = -2Bf C f \varepsilon_f / \text{for heterolayer and } P = -3B_s \varepsilon_s / \text{for substrate with } \varepsilon = \varepsilon_f = (a_f - a_f)/a_f$ is the parallel strain in epilayer and $C_f = (C_{11} - C_{12})/C_{11}$.

Fig. 2 displays our calculated principal bandgap energies at $\Gamma$, L and X high symmetry points for Al$_{1-x}$Ga$_x$N and In$_{1-x}$Ga$_x$N ternary semiconductors in Al$_{1-x}$Ga$_x$N/GaN (left) and In$_{1-x}$Ga$_x$N/GaN (right) heterostructures, respectively, as a function of alloy composition and interface strain. Fig. 2a and b indicate that the interface strain effects on the fundamental bandgaps $\Gamma$, L and X symmetry points in the Al$_{1-x}$Ga$_x$N/GaN (left) and In$_{1-x}$Ga$_x$N/GaN (right) heterostructures can be quite large when the bandgap deformation potential is large. As seen from Fig. 2a and b, the predicted principal bandgaps at $\Gamma$, L and X symmetry points, especially at $\Gamma$ point, are in excellent agreement with experiment [17] in III-N heterostructures. It is gratifying to note that the principal bandgaps of Al$_{1-x}$Ga$_x$N and In$_{1-x}$Ga$_x$N ternaries are nonlinear functions of composition and comparison with experiment indicates that the principal bandgaps can be fitted to the following empirical expression

$$E_{gl}(x) = (1 - x)E_{glAC} + x E_{glBC} - x(1 - x)\Delta E_l$$

(6)

where $\Delta E_l = E_{gl}(AC) - E_{gl}(BC)$ corresponds to the optical bowing coefficient.

As mentioned above, the key property to understand the impact of group III-nitrides based heterostructures on the performance of electronic and optical devices is the composition and strain variation of their energy band structure across the interface. The conduction band offset $\Delta E_c$ and valence band offset $\Delta E_v$ across the interface control the electronic and optical properties of heterostructure devices. Consequently, the reliable and precise modelling of band offsets is crucial in the design and optimization of III-nitride heterostructure devices. Within the with the 2nn sp$^3$s* tight-binding model discussed previously it is easy to determine the band offsets across a Al$_{1-x}$B$_x$C/BC ternary/binary heterointerface once the composition dependent interface strain effects on bandgaps is known. We now determine the magnitude of valence and conduction band offsets at Al$_{1-x}$B$_x$C/BC ternary/binary heterointerface (e.g., Al$_{1-x}$Ga$_x$N/GaN and In$_{1-x}$Ga$_x$N/GaN) according to the following equations [16]:

$$\Delta E_v = \left(\frac{E_v}{\varepsilon_{\infty}}\right)_{BC} - \left(\frac{E_v}{\varepsilon_{\infty}}\right)_{ABC}, \quad \Delta E_{ci} = E_{ciABC} - E_{ciBC} = \Delta E_{gi} - \Delta E_v$$

(7)

where the top of the valence band at $\Gamma$’ symmetry point is $E_v = E_v(\Gamma_{15})$ and the bottom of the conduction band at $\Gamma$, L and X symmetry points are $E_{ci} = E_{i6c}$, $E_{l6c}$ and $E_{X6c}$. 

$E_{cl}(T, P) = E_{cl} + C^0_{cP} T (1 - \ln T) - \frac{a_{cl}}{B} \left[ P - \frac{P^2}{2B} - \frac{(1 + B')P^3}{6B^2} \right]$

(4)

$E_v(T, P) = E_v + C^0_{vP} T (1 - \ln T) - \frac{a_v}{B} \left[ P - \frac{P^2}{2B} - \frac{(1 + B')P^3}{6B^2} \right]$

(5)
Fig. 2. Predicted composition and interface strain effects on bandgap energies of Al$_{1-x}$Ga$_x$N ternary layer grown on GaN buffer (Fig. 2a, on the left) and In$_{1-x}$Ga$_x$N ternary layer grown on GaN buffer compared with experiment [17].

The bandgaps at the $\Gamma$, L and X symmetry points are $E_{g\Gamma} = E_{gL\Gamma}$, $E_{gL}$ and $E_{gX}$. Here $\Delta E_{g\Gamma} = E_{g\Gamma}(ABC) - E_{g\Gamma}(BC)$ with bandgaps $E_{g\Gamma}(ABC)$ and $E_{g\Gamma}(BC)$. $\varepsilon_\infty(ABC)$ and $\varepsilon_\infty(BC)$ are the optical dielectric constants of A$_{1-x}$B$_x$C ternary and BC binary compounds. Shown in Fig. 3 are the calculated conduction and valence band offsets in the Al$_{1-x}$Ga$_x$N/GaN (left) and In$_{1-x}$Ga$_x$N/GaN (right) heterostructures. As shown in these figures, the interface strain effects on conduction band energies in the Al$_{1-x}$Ga$_x$N/GaN (left) and In$_{1-x}$Ga$_x$N/GaN (right) heterostructures can be quite large since the lattice mismatch increases with increase in the alloy composition, especially when the deformation potential of the respective conduction band is large.

5. Conclusion

In this paper we have presented a second nearest neighbour sp$^3$s$^*_{\ast}$ semi-empirical tight-binding model to determine the composition and strain effects on the electronic band structure properties of group III-N semiconductor heterostructures for electronic and photonic applications. The proposed model shows good agreement with experimental results for the bandgap energies and band offsets and has a considerable potential in the design and optimization of group III-N based heterostructures used for the fabrication of electronic and photonic devices.
Fig. 3. Predicted composition and interface strain effects on the valence and conduction band offsets of $\text{Al}_{1-x}\text{Ga}_x\text{N}/\text{GaN}$ (left) and $\text{In}_{1-x}\text{Ga}_x\text{N}/\text{GaN}$ (right) heterostructures.

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