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Computational modeling of novel InN/$Al_{0.30}In_{0.70}N$ multilayer nano-heterostructure

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ABSTRACT

Most of the low dimension heterostructures that have been modeled and simulated to determine various important quantum mechanical parameters are based on GaN/AlGaN and GaAs/AlGaAs. The heterostructures of newly invented material (InN/AlInN), however, have not been well studied. In this paper, novel multilayer nano-heterostructure InN/$Al_{0.30}In_{0.70}N$ of length 288 nm have been modeled and studied to compute the energy band profile within the frame work of eight band **k.p** method, which graphs the energy of conduction and valence band edges versus position, and potential distribution throughout the modeled and one dimensionally simulated nano-heterostructure. In addition, electron–hole densities along with space charge densities have also been calculated for 30% Al concentration. The novelty of the nano-heterostructure due to unusual properties of InN studied by FP-LAPW and LCAO methods is also discussed. The results obtained in this paper will be applicable to the newly invented nano-opto-electronic devices.

1. Introduction

Heterostructures are the building blocks of many of the most advanced semiconductor devices presently being developed and produced. They are essential elements of the highest performance optical sources and detectors and are being employed increasingly in high-speed and high-frequency digital and analog devices. The usefulness of heterostructures is that they offer precise control over the states and motions of charge carriers in semiconductors. For opto-electronic device applications, heterojunction structures play important roles. For example, heterojunction semiconductor lasers are very important light sources for optical communication systems because of minimal dispersion and loss at the wavelengths of 1.30 and 1.55 μm exhibited by optical fiber.

Generally, the heterostructure based devices are based on the energy band structure engineering concept using, for example, a separate-confinement-heterostructure (SCH) quantum well structure to enhance the carrier and the optical confinements, and due to the reason, GaN/AlGaN based heterostructures have recently attracted a good deal of attention for applications in optoelectronic devices operative in UV and visible wavelengths, because of their large bandgap, high breakdown field, and superior thermal conductivity. Nitride based binary and ternary semiconductor compounds having large bandgap are playing very important role in the development and fabrication of short wavelength emitters, photo detectors, and high power frequency transistors [1–6]. Recently, Alvi et al. [7] have investigated energy band profile, potential distribution, electron–hole densities along with space charge densities for simulated model of multilayer nano-heterostructure of GaN/$Al_{0.3}Ga_{0.7}N$. These all parameters have also been found to vary with Al concentration [8].

InN is a material attracting a lot of attention today due to potential device applications. InN was predicted to have the lowest effective mass of electrons among III-nitrides. This may results in high values of carrier mobility and saturation velocity, making InN a promising material for the fabrication of high performance HEMT (high electron mobility transistors), high frequency devices, and full spectrum solar cells [9,10]. The transport parameters of InN almost do not depend on temperature and doping concentration that suggests that InN may have distinct advantages being used in high frequency centimeter and millimeter wave devices. Another possible application of InN is the fabrication of high-speed laser diodes and photodiodes in the optical communication system, although for such devices InN films with p-type of conductivity are necessary. However, sufficient p-type is not realized in InN due to high background donor's concentration [9,11]. Recent progress in growth techniques has led to the fabrication of InN films of improved quality [12].

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It is very difficult task to grow AlInN material due to the large difference existing between InN and AlN covalent bonds, which may lead to phase separation and strong composition inhomogeneities. Moreover, the large difference in optimum growth temperature (T_g) between InN ($\sim$600 °C) and AlN ($\sim$1100 °C) for layers grown by MOVPE does not facilitate the incorporation of Indium in the AlN matrix for Al-rich AlInN layers. Therefore only a few groups worldwide have achieved a reliable material quality [13–18].

Most of the low dimension heterostructures that have been modeled and simulated to determine various important quantum mechanical parameters are based on GaN/AlGaN and GaAs/AlGaAs. The heterostructures of newly invented material (InN/AlInN), however, have not been well studied. In the following sections of this paper, at initial stage, we have calculated energy band structure for InN in WZ and ZB phases obtained from FP-LAPW and LCAO methods. At later stage, we have modeled a novel multilayer nano-heterostructure InN/$Al_{0.30}In_{0.70}N$ and simulated it to determine energy band profile, potential distribution, electron–hole densities along with space charge densities with the help of Nextnano^3 software, that makes use of eight band **k.p** method and incorporates quantum mechanical calculations like the Poisson equation, the Schrödinger equation and determination of wave function, calculation of probability density and charge density.

2. Computational and simulation details

2.1. *k.p* Method

We define **k.p** hemiltonians for wurtzite and zincblende structure of the semiconductors.

For wurtzite, the basic Hamiltonian (without spin–orbit coupling and strain) is defined as

	$s\uparrow$	$s\downarrow$	$x\uparrow$	$y\uparrow$	$z\uparrow$	$x\downarrow$	$y\downarrow$	$z\downarrow$
$s\uparrow$	H_{cc}		H_{cv}					
$s\downarrow$								
$x\uparrow$								
$y\uparrow$				H_{vv}		0		
$z\uparrow$			H_{cv}^T					
$x\downarrow$								
$y\downarrow$				0		H_{vv}		
$z\downarrow$								

$$H_{vv}=\begin{pmatrix} L_1k_x^2+M_1k_y^2+M_2k_z^2 & N_1k_xk_y & N_2k_xk_z \\ N_1k_xk_y & M_1k_x^2+L_1k_y^2+M_2k_z^2 & N_2k_yk_z \\ N_2k_xk_z & N_2k_yk_z & M_3(k_x^2+k_y^2)+L_2k_z^2 \end{pmatrix}$$

the definitions of the parameters L_1, L_2, M_1, M_2, M_3, N_1 and N_2 require that the z-axis is the hexagonal direction of the crystal.

$$H_{cc}=\begin{pmatrix} H_{cc\uparrow} & 0 \\ 0 & H_{cc\downarrow} \end{pmatrix}$$

with

$$H_{cc\uparrow}=H_{cc\downarrow}=\frac{\hbar^2}{2m_0}s_2(k_x^2+k_y^2)+\frac{\hbar^2}{2m_0}s_1k_z^2=\frac{\hbar^2}{2m_0}s_2(k_x^2+k_y^2+k_z^2)+\frac{\hbar^2}{2m_0}(s_1-s_2)k_z^2$$

$$H_{cv}=\begin{pmatrix} H_{cv}^{sx} & H_{cv}^{sy} & H_{cv}^{sz} & 0 & 0 & 0 \\ 0 & 0 & 0 & H_{cv}^{sx} & H_{cv}^{sy} & H_{cv}^{sz} \end{pmatrix}$$

$$H_{cv}^{sx}=B_1k_yk_z+iP_2k_x$$

$$H_{cv}^{sy}=B_2k_xk_z+iP_2k_y$$

$$H_{cv}^{sz}=B_3k_xk_y+iP_1k_z$$

One has additionally to account for the bandoffsets by adding the diagonal matrix:

$$\begin{pmatrix} E_c & & & & & & & \\ & E_c & & & & & & \\ & & E_v+\frac{\hbar^2}{2m}k^2 & & & & & \\ & & & E_v+\frac{\hbar^2}{2m}k^2 & & & & \\ & & & & E_v+\frac{\hbar^2}{2m}k^2 & & & \\ & & & & & E_v+\frac{\hbar^2}{2m}k^2 & & \\ & & & & & & E_v+\frac{\hbar^2}{2m}k^2 & \\ & & & & & & & E_v+\frac{\hbar^2}{2m}k^2 \end{pmatrix}$$

with $K^2=K_x^2+K_y^2+K_z^2$.

The spin–orbit interaction in the basis ($x\uparrow$,$y\uparrow$,$z\uparrow$,$x\downarrow$,$y\downarrow$,$z\downarrow$) is given by

$$H_{SO}=\begin{pmatrix} 0 & -i\Delta_2 & 0 & 0 & 0 & \Delta_3 \\ i\Delta_2 & 0 & 0 & 0 & 0 & -i\Delta_3 \\ 0 & 0 & 0 & -\Delta_3 & i\Delta_3 & 0 \\ 0 & 0 & -\Delta_3 & 0 & i\Delta_2 & 0 \\ 0 & 0 & -i\Delta_3 & -i\Delta_2 & 0 & 0 \\ \Delta_3 & i\Delta_3 & 0 & 0 & 0 & 0 \end{pmatrix}$$

The basis states are expressed explicitly as follows:

$$|u_{hh\uparrow}\rangle=-\frac{1}{\sqrt{2}}|(x+iy)\uparrow\rangle$$

$$|u_{lh\uparrow}\rangle=\frac{1}{\sqrt{2}}|(x-iy)\uparrow\rangle$$

$$|u_{sh\uparrow}\rangle=|z\uparrow\rangle$$

$$|u_{hh\downarrow}\rangle=\frac{1}{\sqrt{2}}|(x-iy)\downarrow\rangle$$

$$|u_{lh\downarrow}\rangle=-\frac{1}{\sqrt{2}}|(x+iy)\downarrow\rangle$$

$$|u_{sh\downarrow}\rangle=|z\downarrow\rangle$$

If we want to include the strain effects we have to add following matrix to H_{vv} as follows:

$$H_{strain}=\begin{pmatrix} l_1\varepsilon_{xx}+m_1\varepsilon_{yy}+m_2\varepsilon_{zz} & n_1\varepsilon_{xy} & n_2\varepsilon_{xz} \\ n_1\varepsilon_{xy} & m_1\varepsilon_{xx}+l_1\varepsilon_{yy}+m_2\varepsilon_{zz} & n_2\varepsilon_{yz} \\ n_2\varepsilon_{xz} & n_2\varepsilon_{yz} & m_3(\varepsilon_{xx}+\varepsilon_{yy})+l_2\varepsilon_{zz} \end{pmatrix}$$

The strain effect on the conduction band (shift of the conduction band) is described by the absolute deformation potential for the conduction band a_c

$$E_c\rightarrow E_c+a_c tr(\varepsilon)$$

For zincblende, the basic Hamiltonian (without spin–orbit coupling and strain) is defined as

	$s\uparrow$	$s\downarrow$	$x\uparrow$	$y\uparrow$	$z\uparrow$	$x\downarrow$	$y\downarrow$	$z\downarrow$
$s\uparrow$	H_{cc}		H_{cv}					
$s\downarrow$								
$x\uparrow$								
$y\uparrow$				H_{vv}		0		
$z\uparrow$			H_{cv}^T					
$x\downarrow$								
$y\downarrow$				0		H_{vv}		
$z\downarrow$								

$$H_{vv}=\begin{pmatrix} Lk_x^2+M(k_y^2+k_z^2) & Nk_xk_y & Nk_xk_z \\ Nk_xk_y & Lk_y^2+M(k_x^2+k_z^2) & Nk_yk_z \\ Nk_xk_z & Nk_yk_z & M(k_x^2+k_y^2)+Lk_z^2 \end{pmatrix}$$