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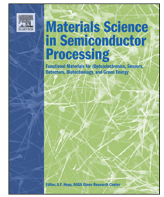

Composition dependence of the band offsets in wurtzite nitride-based heterojunctions

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ABSTRACT

We theoretically calculate the composition dependence of the valence- and conduction- band discontinuities at the interfaces between selected III-nitride ternary materials with wurtzite structure, e.g. $Al_xGa_{1-x}N/Al_xGa_{1-x}N$, $In_xGa_{1-x}N/In_xGa_{1-x}N$ and $In_xA_{1-x}N/In_xA_{1-x}N$. Calculations are performed using a theoretical model, initially proposed by Chuang et al. 1997 [1]. Depending on a particular set of input parameters, simulation results show that band offsets change more or less with strain. The valence band offsets, together with the resulting conduction band offsets, indicate that a type-I, type-II band line-up forms at $In_xGa_{1-x}N$/GaN, $Al_xGa_{1-x}N$/GaN heterojunctions with varying In, Al contents respectively. Also, based upon the same model, we propose a type I Indium-dependent band alignment in $In_xAl_{1-x}N$/AlN interfaces. The failure of the transitivity rule, which is often used to determine the band offsets in heterojunctions, was demonstrated and its cause was explained. The obtained results are well compared with experiment and theory in various reliable test cases and therefore provide a basis for optimization and design of novel interface structures.

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1. Introduction

The group III-nitrides and their alloy systems are emerging as the important class of semiconductor compounds for optoelectronic and electronic applications. Since the demonstration of high-efficiency InGaN blue LEDs by Nakamura et al. [2], nitrides have found their way into many commercial optoelectronics device applications. Large progress on the growth of devices based on such materials was achieved and a great interest is given to the realization of quantum devices using GaN-based material. Indeed, AlN, GaN, InN and their alloys AlGaN, InGaN and InAlN, have attracted immense attention owing to their outstanding properties such as wide band-gap energy, high peak electron velocity, high saturation electron velocity, and high thermal stability [3,4].

The band gap energy of InGaN, ranging from the near infrared (0.7 eV) to the ultraviolet (3.4 eV), makes such alloy a promising candidate for radiation-resistant multi-junction solar cells [5,6]. In $_xAl_{1-x}N$ is attracting more and more attention for its interesting characteristics, in particular, (i) it covers a large bandgap energy range spanning from the deep infrared to the far ultraviolet and (ii) it can be in-plane lattice matched to GaN with In composition around $x = 0.18$. Thus, $In_xAl_{1-x}N$ is holding much potential for use in a variety of optoelectronic and electronic device applications such as distributed Bragg reflectors and high-electron mobility transistors. Furthermore, III-nitride semiconductors are characterized by a large conduction band discontinuity (1.75 eV between GaN and AlN [7]), which makes GaN/AlGaN heterostructures of great interest for intersubband optoelectronics both in the near infrared and in the terahertz spectral ranges. Thanks to the high energy of their longitudinal optical phonon modes (92 meV in GaN), III-nitrides are excellent candidates for the fabrication of high temperature THz quantum cascade lasers QCLs [6].

Under ambient conditions, the thermodynamically stable structure for bulk AlN, GaN, InN and their ternaries along with the quaternary is wurtzite (wz). Furthermore, wz group-III nitrides are piezoelectric, in which large spontaneous polarizations exist along the *c* axis (polar axis). Moreover, depending on the degree of lattice mismatch, the piezoelectric effect also contributes to the polarization fields to a certain extent. The discontinuity of polarization across a heterojunction manifests itself as fixed interface bound polarization charges and induces the "built-in electric field", which is a vital parameter in determining bandgaps, band structure and other electronic properties [8,9]. For transport modelling, of a whole multilayered device stack, such "built-in electric field" is generally treated within Schrödinger–Poisson-transmittance models [10].

To manipulate the electrical, optical, and transport properties in nitride based devices effectively, an accurate determination of

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the basic properties of wurtzite nitride based heterostructures is crucial. The valence band offset (VBOs) and conduction band offsets (CBOs) between two alloys are the key parameters to the design heterostructures- based, $Al_xGa_{1-x}N$, $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$ optoelectronic devices. In fact, a precise knowledge of the latter quantities is vital for evaluating the degree of the localization of charges at the interfaces of semiconductor multilayers, the degree of carrier confinement and therefore the usefulness of the material for device applications.

Experimental [11–14] and theoretical [1,15–28] methods have been a serious challenge in determining valence and conduction band offsets of semiconductor heterojunctions. The authors of reference [1] have proposed a theoretical model for calculating the band structure of strained quantum well wurtzite semiconductors including strain effects on the shifts of band edges. They have applied their model for the calculation of GaN/AlGaN band offset heterojunction. Information about band offsets at further homovalent and heterovalent [29,30] wurtzite nitride heterojunctions is still lacking. This has inspired us to perform and update band offset calculations, using the model detailed in reference [1], at variety of wurtzite nitride based interfaces with taking advantage of the outcomes of recent improvements in epitaxial growth of III-nitrides.

The organization of the present paper is as follows. In Section 2, we describe the intended theoretical model and we give the computational details of the band offset calculations. In Section 3, we calculate the band offsets and the strained band gaps of the considered heterojunctions $Al_xGa_{1-x}N/Al_yGa_{1-y}N$, $In_xGa_{1-x}N/In_yGa_{1-y}N$ and $In_xA_{1-x}N/In_yA_{1-y}N$ and their dependence on aluminum and indium compositions respectively. In Section 4, we focus on the discussion of the obtained results. Finally, Section 5 summarizes the present work.

2. Theoritical background

2.1. Band edge energies

We consider a wurtzite strained interface (material-1/material-2), pseudomorphically grown along the (0001) (c-axis) direction. We note that practical growth of such structure is only possible for layers that do not exceed a certain critical thickness which depends on the material and on the degree of lattice mismatch [23]. To predict the band lineup at strained interfaces, the first step is to obtain values of the band lineups at ideal interfaces and after one must include the appropriate strain in each of the materials to construct a pseudomorphic interface [23].

In contrast to zinc blend materials, the wurtzite structure does not give a triply degenerate valence band edge [31]. For the unstrained system, the HH and LH bands are doubly degenerate and the CH band is split off by the crystal field splitting Δ_1 which is in general not related to the spin orbit interaction [31]. In principle, two different spin orbit splitting parameters exist (Δ_2 and Δ_3); they are commonly assumed equal and are allied to the spin orbit splitting Δ_{so} by the following relation:

$$\Delta_2 = \Delta_3 = \frac{\Delta_{so}}{3} \tag{1}$$

Consequently, adding the spin orbit interaction to the crystal field effect, the valence band-edge energies for strain free wurtzite semiconductor layers are given, with respect to reference energy E_v^0 by [1]

$$E_{iv,1}^{uns} = E_v^0 + \Delta_1 + \Delta_2 \tag{2-a}$$

$$E_{iv,2}^{uns} = E_v^0 + \frac{\Delta_1 - \Delta_2}{2} + \sqrt{\left(\frac{\Delta_1 - \Delta_2}{2}\right)^2 + 2\Delta_3^2} \tag{2-b}$$

$$E_{iv,3}^{uns} = E_v^0 + \frac{\Delta_1 - \Delta_2}{2} - \sqrt{\left(\frac{\Delta_1 - \Delta_2}{2}\right)^2 + 2\Delta_3^2} \tag{2-c}$$

where i denotes the semiconductor material (1 or 2) and the subscripts 1, 2 and 3 in $E_{iv,1}^{uns}$, $E_{iv,2}^{uns}$ and $E_{iv,3}^{uns}$ stand for heavy hole (HH), light hole (LH) and crystal field split off (CH) respectively.

The lattice constant mismatch between the material (1 or 2) and the substrate gives rise to a strain in the layer described by the following equations:

$$\varepsilon_{xx} = \varepsilon_{yy} = \frac{a_0 - a}{a} \tag{3-a}$$

$$\varepsilon_{zz} = -\frac{2C_{13}}{C_{33}}\varepsilon_{xx} \tag{3-b}$$

where a_0 and a are the lattice constants of the substrate and the strained material respectively. C_{ij} designate the elastic constants.

We note that for wurtzite structures, the valence-band-mixing between the three valence bands (heavy hole (HH), light hole (LH) and crystal field split off (CH)), strongly coupled, and has to be taken into account with the aim to take full advantage of the strained structure and to obtain better designs [1]. In fact, the strain affects the valence band edges and so influences the band discontinuity at the strained layer interfaces. According to reference [1], under strain, the valence band edge-energies are given by

$$E_{iv,1}^{str} = E_v^0 + \Delta_1 + \Delta_2 + \theta_\epsilon + \lambda_\epsilon \tag{4-a}$$

$$E_{iv,2}^{str} = E_v^0 + \frac{\Delta_1 - \Delta_2 + \theta_\epsilon}{2} + \lambda_\epsilon + \sqrt{\left(\frac{\Delta_1 - \Delta_2 + \theta_\epsilon}{2}\right)^2 + 2\Delta_3^2} \tag{4-b}$$

$$E_{iv,3}^{str} = E_v^0 + \frac{\Delta_1 - \Delta_2 + \theta_\epsilon}{2} + \lambda_\epsilon - \sqrt{\left(\frac{\Delta_1 - \Delta_2 + \theta_\epsilon}{2}\right)^2 + 2\Delta_3^2} \tag{4-c}$$

$$\lambda_\epsilon = D_1\varepsilon_{zz} + D_2(\varepsilon_{xx} + \varepsilon_{yy}) \tag{5}$$

$$\theta_\epsilon = D_3\varepsilon_{zz} + D_4(\varepsilon_{xx} + \varepsilon_{yy}) \tag{6}$$

we note that λ_ϵ and θ_ϵ depend on the deformation potentials $D_{1,2,3,4}$.

The procedure outlined above for valence bands also applies for conduction bands. In strained free semiconductor system, the conduction band edge E_{ic}^0 is above the top valence band with band gap energy E_g. Adding strain effects, the conduction band edge has an hydrostatic energy shift $P_{c\varepsilon}$:

$$E_{ic} = E_{ic}^0 + P_{c\varepsilon} \tag{7}$$

$$P_{c\varepsilon} = a_{cz}\varepsilon_{zz} + a_{ct}(\varepsilon_{xx} + \varepsilon_{yy}) \tag{8}$$

We note that a_{cz} and a_{ct} are the conduction band deformation potentials which are usually assumed to be equal for simplicity [1] and are generally combined with the valence band deformation potentials D_1 and D_2 respectively [32].

2.2. Band offsets

The valence ($\Delta E_{v,1,2,3}^{str}$) and conduction (ΔE_c^{str}) band discontinuities of an heterojunction (material-1/material-2) may then be estimated by the difference between the individual band-edge energies of the strained materials (material 1and material 2) and

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