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Review

Impact of strain on the band offsets of important III–V quantum wells: $In_xGa_{1-x}N$/GaN, GaAs/$In_xGa_{1-x}P$ and $In_xGa_{1-x}As$/AlGaAs

Dipankar Biswas*, Partha Pratim Bera, Tapas Das, Siddhartha Panda

Institute of Radiophysics and Electronics, University of Calcutta, 92 Acharya Prafulla Chandra Road, Kolkata 700009, India

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ABSTRACT

Lattice strain has immense effect on the optoelectronic properties of III–V semiconductor quantum wells (QWs), since it introduces a pronounced change on the band properties of QWs and it is often purposefully introduced to improve device performance. In this paper we report the results of our experimental and theoretical studies on, how the important parameter, the band offset, changes with strain for $In_xGa_{1-x}N$/GaN, GaAs/$In_xGa_{1-x}P$ and $In_xGa_{1-x}As$/AlGaAs QWs. Experimentally the band offsets have been studied through capacitance transient measurements in the form of deep level transient spectroscopy (DLTS) on suitable QWs within a Schottky diode. The energy levels in a QW are considered to be analogous to a deep trap in the forbidden energy gap. From detailed balance between the emission and capture, Arrhenius type expressions were derived to analyze transient emission data, from which the band offsets were computed. Theoretically the band positions at the heterointerfaces have been calculated from the equations developed, which directly correlate the position of the bands with the strain at the interface. The strain is calculated from the In mole fractions and lattice constants. The parameters implicitly involved are the elastic stiffness constants (C_{11} and C_{12}), the hydrostatic deformation potential of the conduction band (a'), the hydrostatic deformation potential (a) and the shear deformation potential (b) for the valance band. The results should be useful to research workers in the field of optoelectronics.

Contents

* Corresponding author. Tel.: +91 33 2350 9413; fax: +91 33 2351 5828.
E-mail address: diiibiswas@yahoo.co.in (D. Biswas).

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1. Introduction

One of the most important parameters for the design of heterojunction and quantum well electronic and optoelectronic devices is the heterojunction band offset. The band offset not only depends on the semiconductor materials forming a heterojunction but it also depends on the interfacial strain caused by lattice mismatch. In this paper we present our rigorous studies on, how the band offsets of three vitally important III–V quantum wells (QWs) $In_xGa_{1-x}N$/GaN, GaAs/$In_xGa_{1-x}P$ and $In_xGa_{1-x}As$/AlGaAs, vary with strain.

The ternary compound semiconductor $In_xGa_{1-x}N$ has a direct band gap from 0.7 to 3.4 eV at room temperature and an extremely large heterojunction band offset, which makes the material highly successful and promising for light emission around the blue–green range [1]. Its heterostructures offer a high band offset for successful carrier confinement. Relations for computing the band lineups of $In_xGa_{1-x}N$ based heterostructures have been developed. The band positions for $In_xGa_{1-x}N$/GaN heterointerfaces are calculated from the equations developed [2], which directly correlate the positions of the bands with the band gap of InN and strain at the interface. The strains are calculated from the In mole fractions and lattice constants. The parameters implicitly involved are, the elastic stiffness constants (C_{11} and C_{12}), the hydrostatic deformation potential of the conduction band (a'), and the hydrostatic deformation potential (a) and shear deformation potential (b) for the valence band. Computations have been carried out for different reported band gaps of InN. The effects of strain become prominent as the mole fraction of In increases, changing the band offset ratios. The obtained results have been established by comparison with experimental results reported for the annealing of $In_{0.23}Ga_{0.77}N$/GaN multiple quantum wells (MQWs) [3].

The lattice matched GaAs/$In_{0.49}Ga_{0.51}P$ heterojunction emerged as an important alternative to the GaAs/AlGaAs system for potential application to modulation doped field effect transistors. In particular, Al can be avoided for high quality quantum devices, using this heterointerface. The heterojunction is believed to have a valence band offset ΔE_v larger than the conduction band offset ΔE_c, which makes it attractive also for logic applications. In our pioneering report we established this, experimentally, through capacitance–voltage transient measurements in the form of deep level transient spectroscopy (DLTS) [4]. The band offsets were found to be $\Delta E_c = 0.198$ eV and $\Delta E_v = 0.285$ eV. There was a recent contradiction and again we reestablished the band offsets theoretically [5].

Beside other applications, the strained QW InGaAs/AlGaAs laser has found immense importance in connection with Er-doped fiber amplifier. This important heterojunction has been studied experimentally through DLTS measurements and optical DLTS measurements on single and double QWs. Thus the conduction band offset and the valence band offset were measured separately to obtain accurate results. The effect of strain was studied, varying the In mole fraction. The detail of the process is discussed in the paper [6].

This paper will present the methodologies and the results of how the band offsets of the three QWs change with strain, along with suitable discussions.

2. $In_xGa_{1-x}N$/GaN QWs

The effect of strain is very strong in the $In_xGa_{1-x}N$/GaN QWs. Besides changing the optical properties, it introduces very strong piezoelectric fields in the QWs which increase with In mole fraction and strain. Therefore, the investigation of the change of the band lineup with the strain seems worthwhile. To determine the band lineup of the heterointerface of the strained layer, the energy shift due to the effect of strain needs to be calculated, since the electron and hole recombination occurs from the final energy states that are altered by the effect of strain.

For model calculations we have considered an $In_xGa_{1-x}N$/GaN system in which the composition of In has been varied, to change the strain. Indium mole fraction (x) is varied from 0 to 1.0, that is, from the lattice matched GaN/GaN system to the highly strained InN/GaN system through the strained $In_xGa_{1-x}N$/GaN system. The strain of $In_xGa_{1-x}N$/GaN is calculated from the equation [7]

$$\varepsilon = (d_e - d_s)/d_s, \tag{1}$$

where d_e and d_s are the lattice constants of the epitaxial layer and the substrate, respectively. The variation of strain with In mole fraction is shown in Fig. 1. The strain varies almost linearly with the mole fraction of In. The energy correction due to the strain for the conduction band and valence band are given by the formulas [8],

$$\Delta E_{srt,c} = 2a'[(C_{11} - C_{12})/C_{11}]\varepsilon, \tag{2}$$

$$\Delta E_{srt,v} = 2a[(C_{11} - C_{12})/C_{11}]\varepsilon + b[(C_{11} + C_{12})/C_{11}]\varepsilon, \tag{3}$$

where a' is the hydrostatic deformation potential of the conduction band, C_{11} and C_{12} are the elastic stiffness constants, and a and b are the hydrostatic deformation potential and shear deformation potential for the valence band, respectively. To investigate the effect of strain on the band lineup the energy correction terms as represented in Eqs. (2) and (3) have been included. The parameters used in this paper are taken from Vurgaftman and Meyer [9]. Linear interpolation has been used to calculate d_e, a', a, and b of the ternary materials and the interpolation has been weighted by the lattice constant for calculating C_{11} and C_{12} of ternary materials.

Figs. 2 and 3 show the variations of the conduction band lineups and valence band lineups with strain, respectively, for different reported band gaps of InN [2]. From the figures we have extracted suitable expressions for calculation of the band positions of $In_xGa_{1-x}N$/GaN with strain within a maximum error bar of $\pm 2.5\%$, as expressed below

$$E_c = 3.39478 + (-0.29077 + 0.03872E_{g,\mathrm{InN}} + 0.00512E_{g,\mathrm{InN}}^2)\varepsilon + 0.0092\varepsilon^2, \tag{4}$$

$$E_v = 0.00153 + (0.14508 - 0.03997E_{g,\mathrm{InN}} - 2.49713 \times 10^{-4}E_{g,\mathrm{InN}})\varepsilon - 0.00363\varepsilon^2, \tag{5}$$

where E_c and E_v are the conduction band and valence band positions, respectively, and $E_{g,\mathrm{InN}}$ is the band gap energy of InN. The strain ε is expressed in percentage (%).

The variations of conduction and valence band lineups with In mole fraction, as emerges from Eqs. (4) and (5) are