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Calculations for the band lineup of strained $In_xGa_{1-x}N/GaN$ quantum wells: Effects of strain on the band offsets

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Band lineup is one of the most important parameters associated with carrier confinement in heterostructures. 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, which directly corelate 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 ratio. © *2009 American Institute of Physics*.
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In the recent past, strained quantum wells (QWs) have attracted the interest of many researchers working in the semiconductor optoelectronic area particularly in the field of lasers. A large variety of quantum structures have been created. Among them, strained QWs have exhibited many interesting phenomena. Attractive possibilities of strained QWs have been proposed and demonstrated.[1–3] Higher optical gain[4] and very large modulation band widths[5,6] have been obtained by using QWs with compressive strain. Polarization-insensitive optical gains have been obtained through the use of tensile strained QWs.[7,8]

During growth and processing, nanostructures are likely to undergo several periods of high temperature thermal cyclings. Due to intermixing and redistribution of the composition, strain and band lineups of the QWs are likely to change, leading to changes in the optical properties.[9,10] Band lineup of semiconductor heterointerfaces is one of the most dominant parameters which determines the optoelectronic properties of heterojunctions. In spite of numerous experimental and theoretical studies[11] the underlying principles that govern the alignment of the bands are still debatable. Especially the relative importance of bulk versus surface or interface properties is still not absolutely settled.

To determine the band lineup of the heterointerface of strained layers, the energy shift due to the effect of strain needs to be calculated, since the electron-hole recombination occurs from the final energy states that are altered by the effect of strain. Although there are several possible methods to calculate the valence band edge (E_{Vo}) of InGaAs/InP, InGaAsP/InP,[12] and InSe/GaSe (Ref. 13) systems, calculations of the band lineup of InGaN/GaN systems have not been widely discussed.

The ternary compound semiconductor $In_xGa_{1-x}N$ has a direct band gap from about 2.1 to 3.4 eV, which makes it suitable for emission in the blue-green range.[14] Its heterostructures offer a high band offset for successful carrier confinement. Therefore, the investigation of change of band lineup with strain and their effects on the optical properties of $In_xGa_{1-x}N/GaN$ interfaces seem worthwhile. In this communication we determine theoretically the band lineup of $In_xGa_{1-x}N/GaN$ systems with strain for different reported values of the band gaps of InN.

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 lattice matched GaN/GaN system to highly strained InN/GaN system through strained $In_xGa_{1-x}N/GaN$ system. The strain of $In_xGa_{1-x}N/GaN$ is calculated from the equation[12]

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

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 mole fraction of In. The energy correction due

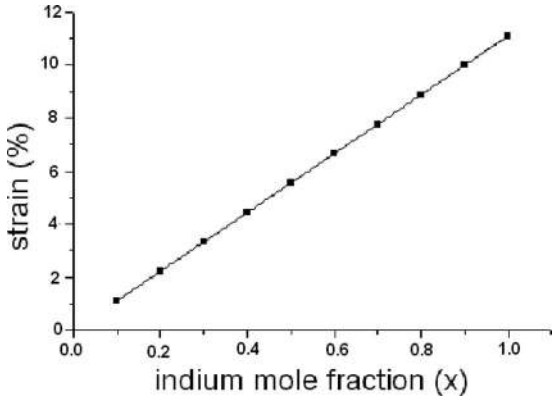

FIG. 1. Variation of strain with indium mole fraction in an $In_xGa_{1-x}N/GaN$ system.

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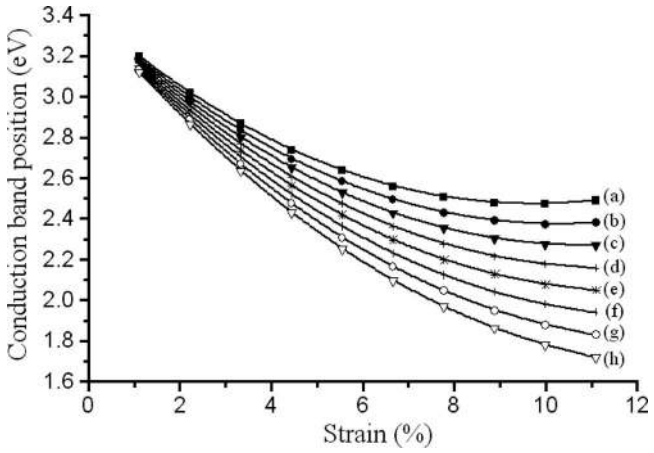

FIG. 2. Variations of conduction band positions with strain. Band gap of InN ($E_{g,\mathrm{InN}}$) is varied as (a) 2.1 eV, (b) 1.9 eV, (c) 1.7 eV, (d) 1.5 eV, (e) 1.3 eV, (f) 1.1 eV, (g) 0.9 eV, and (h) 0.7 eV.

to strain for the conduction band and valence band are given by the formulas[15]

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

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

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 we have to include the energy correction terms as represented in Eqs. (2) and (3). The parameters used in this paper are taken from Vurgaftman and Meyer.[16] 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.

Figures 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 ($E_{g,\mathrm{InN}}$), that

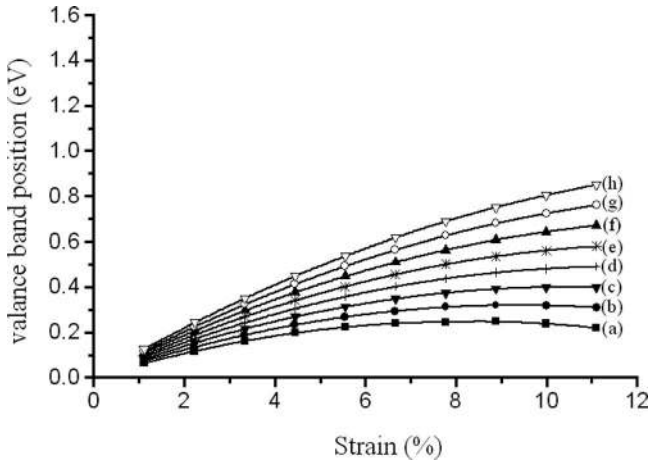

FIG. 3. Dependence of valence band positions on strain. Band gap of InN ($E_{g,\mathrm{InN}}$) is varied as (a) 2.1 eV, (b) 1.9 eV, (c) 1.7 eV, (d) 1.5 eV, (e) 1.3 eV, (f) 1.1 eV, (g) 0.9 eV, and (h) 0.7 eV.

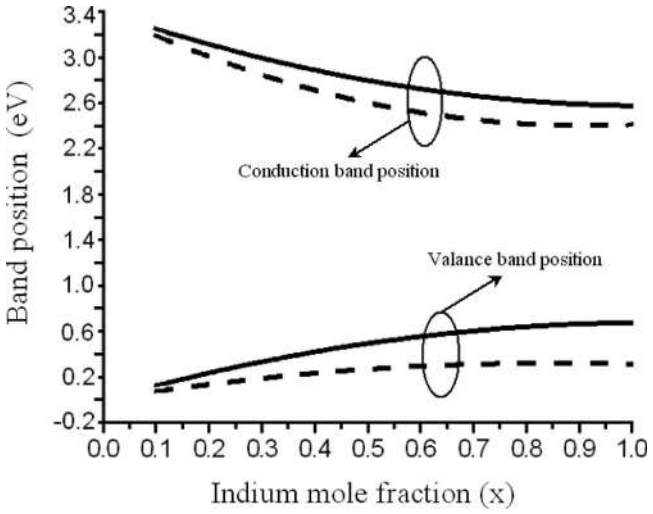

FIG. 4. Band positions of $In_xGa_{1-x}N/GaN$ system. The continuous curves show the variation without considering strain and the dashed curves show the variation considering strain.

is, 0.7–2.1 eV.[17–26] From Figs. 2 and 3, 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:

$$E_c = 3.394\ 78 + (-0.290\ 77 + 0.038\ 72E_{g,\mathrm{InN}} + 0.005\ 12E_{g,\mathrm{InN}}^2)\varepsilon + 0.009\ 92\varepsilon^2, \tag{4}$$

$$E_v = 0.001\ 53 + (0.145\ 08 - 0.039\ 97E_{g,\mathrm{InN}} - 2.497\ 13 \times 10^{-4}E_{g,\mathrm{InN}}^2)\varepsilon - 0.003\ 63\varepsilon^2, \tag{5}$$

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 calculated from Eqs. (4) and (5) are shown in Fig. 4. For computation a typical value of band gap of InN, 1.9 eV, is considered. For a comparative study we have also plotted the same variation without considering strain. It is clear from the variation that the strain lowers the band positions, i.e., conduction band offset increases and valence band offset decreases with strain, which means that if we have an InGaN/GaN QW of high In content, the well of the conduction band will be deeper and that of the valence band will be shallower due to the effect of strain.

Recently photoluminescence (PL) results on annealing of $In_{0.23}Ga_{0.77}/GaN$ multi-QWs (MQWs) of 30 Å widths have been reported by Chuo *et al.*[27] The as grown samples were subjected to thermal annealing in quartz tube furnace at different temperatures ranging from 950 to 1050 °C in nitrogen ambient for 10–40 min. The experimental and theoretical curves of PL peak energies against annealing time at 950 and 1000 °C for MQW structure are shown in Fig. 5. With our newly developed band lineup model the data could be fitted to within 1% average error.

Reported values of the ratios of conduction band offset to valence band offset for $In_xGa_{1-x}N/GaN$ QW structures, $\Delta E_c : \Delta E_v$, vary widely from 38:62 to 83:17.[9] From this work

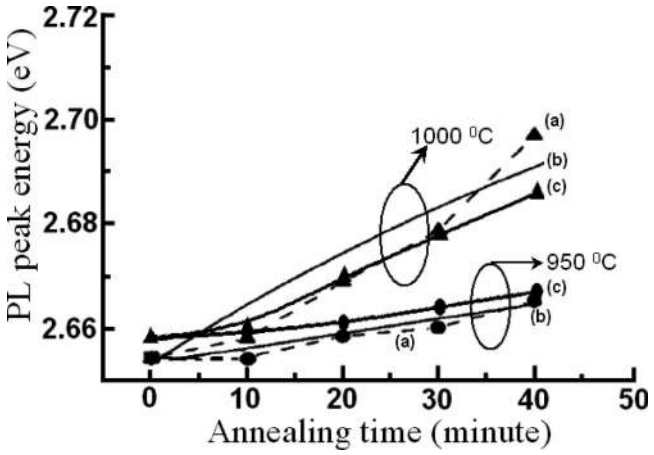

FIG. 5. Variation of PL peak energy with annealing time (a) found experimentally, (b) calculated by Chuo *et al.*, and (c) calculated using Eqs. (4) and (5).

a conclusion seems plausible that the band offset ratio is around 68:32 and it changes with the In mole fraction.

To summarize, in this paper we have presented the procedures for calculating the band lineups of $In_xGa_{1-x}N/GaN$ systems as a function of In mole fraction, strain, and band gap of InN. A comparative study of band lineups with and without strain has been presented. It is observed that strain lowers the band positions. When strain is not considered for the calculation of band lineups, the band offset ratio remains constant. On the other hand the band offset ratio changes if we consider the effect of strain. Strain increases the conduction band offset and decreases the valence band offset. This means that for an $In_xGa_{1-x}N/GaN$ system due to the strain, the well corresponding to the conduction band will be deeper and the well corresponding to the valence band will be shallower.

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