

Strain Effect on InGaN/GaN Quantum Well

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ABSTRACT: The strains are calculated from the In mole fraction and lattice constants. The parameters implicitly involved are elastic stiffness constants (C11 and C22), the hydrostatic deformation potential of the conduction band (a') and the hydrostatic deformation potential (a) and shear deformation potential (b) for the valence band. The effects of strain become prominent as the mole fraction of In increases, changing the band effect ratio. Different levels of strain energy were built with different quantum well widths. An increase in the quantum well width by only one monolayer can result in a large reduction in the transition energy.

KEYWORDS: Quantum Well, transition energy, redshift, built-in-electric field, spontaneous polarization, piezoelectric polarization.

I. INTRODUCTION

Recent years, there has been great interest in group III-nitrides because they have direct, large bandgap materials ranging from infrared to ultraviolet [1]. Optical devices with InGaN/GaN materials system have been widely investigated. Due to the large lattice mismatch between InN and GaN, there is a large polarization field along [0001] orientation in the InGaN quantum wells grown on thick GaN [5-9]. Therefore the optical properties of [0001]-oriented InGaN strained quantum wells are strongly affected by polarization fields. The large internal fields not only cause a redshift but also separate the wave function of the holes and electrons in the InGaN/GaN quantum well [3].

In this paper we calculate strain and built-in electric field which is built due to the spontaneous and piezoelectric polarization and compared with experimental data reported recently by another group. We also calculate transition energy variation with strain or InGaN/GaN quantum well.

II. THEORETICAL DETAILS

In this calculation we consider a thin InGaN well layer coherently grown on a thick GaN layer along [0001] and then an InGaN well layer. When an InGaN layer is grown on a thick GaN layer, the strain of the InGaN layer varies with different In mole fraction and different growth.

The total polarization in the GaN layer is simply the sum of the spontaneous and piezoelectric polarization

$$P = P^{SP} + P^{PZ} \quad (1)$$

The spontaneous polarization of the random ternary group III-nitride alloys is given to second order in x by (in C/m²)

$$P_{InGaN}^{SP}(x) = P_{InN}^{SP}x + P_{GaN}^{SP}(1-x) + 0.037x(1-x) \quad (2)$$

The values of P_{InN}^{SP} and P_{GaN}^{SP} are negative.

$$(P_{InN}^{SP} = -0.042 \text{ C/m}^2 \text{ and } P_{GaN}^{SP} = -0.034 \text{ C/m}^2)$$

The piezoelectric polarization of InGaN is

$$P_{InGaN}^{PE} = P_Z = 2 \frac{a_{GaN} - a_{InGaN}}{a_{InGaN}} \left(e_{31} - e_{33} \frac{c_{13}}{c_{33}} \right) \quad (3)$$

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Since $(e_{31}-e_{33}*c_{13}/c_{33}) < 0$ is valid for InGaN over the whole range of composition from equation (3), we can conclude that the piezoelectric polarization is positive for a compressively strained InGaN layer grown on thick GaN with Ga face polarity and as a consequence, the orientation of the piezoelectric and spontaneous polarization are antiparallel in this case.

The built in electric field F^{InGaN} in the InGaN layer and F^{GaN} in the GaN barrier layer between the two coupled quantum wells as follows.^[2]

$$F^{InGaN} = - \frac{(P_{SP}^{InGaN} + P_{PE}^{InGaN} - P_{SP}^{GaN})L^{GaN}}{\epsilon_0(2\epsilon_e^{GaN}L^{InGaN} + \epsilon_e^{InGaN}L^{GaN})} \dots\dots\dots(4)$$

$$F^{GaN} = 2 \frac{(P_{SP}^{InGaN} + P_{PE}^{InGaN} - P_{SP}^{GaN})L^{InGaN}}{\epsilon_0(2\epsilon_e^{GaN}L^{InGaN} + \epsilon_e^{InGaN}L^{GaN})} \dots\dots\dots(5)$$

The direction of the built-in electric field F depends on the orientation of the piezoelectricity and spontaneous polarization and can be determined by both the polarity of the crystal and strains of the QW structures [4]. We will consider wurtzite $In_xGa_{(1-x)}N/GaN$ quantum heterostructures grown along the [0001] direction(c-axis) of the bulk materials. Furthermore, we choose the x-axis along this direction. In this case, the direction of the piezoelectricity and spontaneous polarization is along the x direction [3]. Hence the built-in electric field F arising from spontaneous polarization and from the piezoelectric effect is in the direction of the x axis.

We calculate the built-in electric field of the QW structure, which is extremely strong, of the order of MV/cm. The strong electric field will induce a remarkable modification of the band edges[1]. Thus, the as-grown InGaN/GaN QW structure is trapezoidal shape.

III. RESULTS AND DISCUSSION

Figure(1) shows that band gap energy increases with increasing indium mole fraction. Band gap energy also depends upon bowing parameter and band gap energy of InN and GaN.

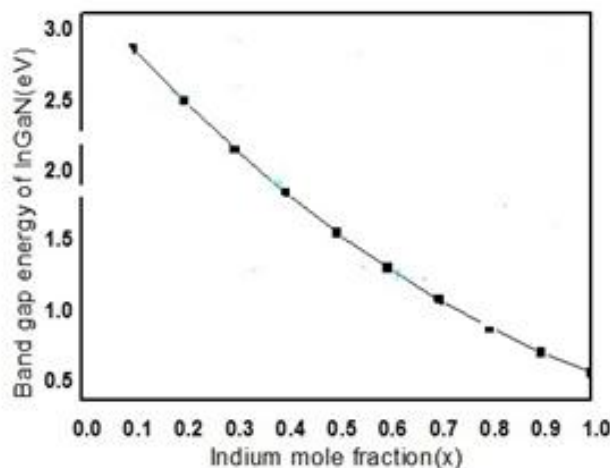


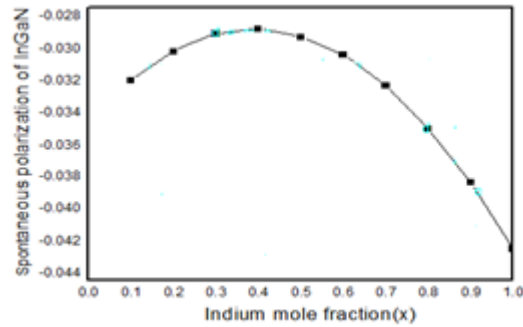
Fig. 1. Represent the graph between bandgap energy of InGaN and indium mole fraction

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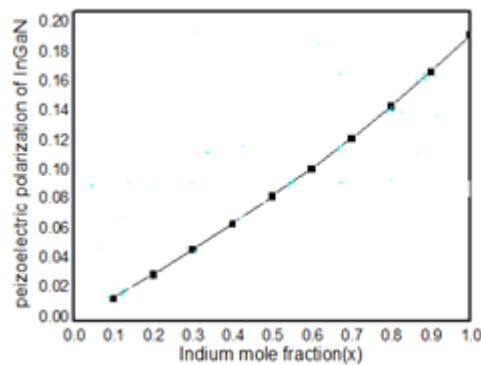
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Figure(2) shows that spontaneous polarization of InGaN is increases with indium mole fraction upto indium
Fig2. Represent the graph between spontaneous polarization of InGaN and indium mole fraction



Figure(3) shows that piezoelectric polarization is increases with increasing indium mole fraction.This
polarization create due to strain.

Fig 3. Represents the graph between piezoelectric polarization of InGaN and indium mole fraction

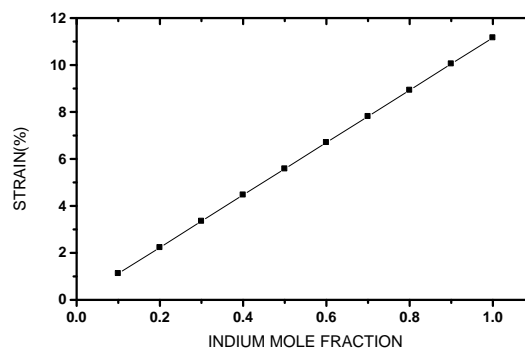


Fig 4. Represents the graph between strain and indium mole fraction

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Figure(4) shows that strain is increases with increasing mole fraction. More strain generates more electric field, that changes the profile of quantum well. The built-in-electric field also changes the transition energy of InGaN/GaN quantum well.

IV. CONCLUSION

The strains are calculated from the In mole fraction and lattice constants. The built-in-electric generates due to strain in quantum well. The effects of strain become prominent as the mole fraction of In increases, changing the band effect ratio different level of strain energy were built with different quantum well width. An increase in the quantum well width by only one monolayer can result in a large reduction in the transition energy. Strain generates built-in-electric field and that filed changes band profile that also changes transition energy.

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