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Simulation Study of GaN/$Al_{1-x}Ga_xN$ Quantum Well (QW) Operating in the UV Region

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ABSTRACT: *This study describes the characteristics of GaN/$Al_{1-x}Ga_xN$ quantum well (QW) operating in the UV region by varying different parameters. It is well known that the spontaneous and piezoelectric polarisations in wurtzite nitride heterostructures give rise to large built-in electric fields, which leads to an important consequence in the optical properties of GaN/$Al_{1-x}Ga_xN$ quantum wells. We first modelled the effect of electric field on the calculated electronic band structure. The increase in electric field affected the band structure for a fixed QW and barrier thickness. Then we investigated the effect of QW thickness on the bandgap energy for different electric fields. Afterwards, the Al composition (1-x) and $Al_{1-x}Ga_xN$ barrier thickness are varied for different well thickness with a fixed electric field.*

Keywords: GaN QW, QW thickness, $Al_{1-x}Ga_xN$ barrier, UV region

1. INTRODUCTION

Group III-nitride semiconductors mainly AlN, GaN, InN and their alloys have attracted a lot of attention in the past decade due to their applications in short wavelength light emitters and many optoelectronic devices.[1,3] In particular, as an UV emitter, both GaN quantum dots (QDs) and quantum wells (QWs) embedded in AlN or $Al_{1-x}Ga_xN$ barrier seem to be a promising candidate for many applications.[4,6] However, in nitrides the grown wurtzite phase introduces spontaneous polarisation. In addition, a strain induced piezoelectric polarisation arises due to the lattice mismatch of the hetero structures.[7] This combined polarisation has a detrimental effect in nitride materials. For instance, in nitride QWs and QDs, the polarisation difference between well or dot and barrier exhibits interfacial charge accumulation. Therefore, a strong electric field appears on the order of several MV cm^{-1}.[7,8] This strong electric field in wells and dots exhibit low internal quantum efficiency, a phenomenon of quantum-confined Stark effect (QCSE) which creates a spatial separation of electrons and holes in the quantum structure. The large spatial separation of electrons and holes leads to the increase of radiative recombination time.[9]

To reduce the electric field, the epitaxial layer can be grown on semipolar and nonpolar substrates. Moreover, several other attempts were taken such as band structure engineering of QW region and matching the polarisation of the active QW and QD layers, using a ternary or quaternary nitride barrier.[10,11] It is reported that the GaN quantum structure shows red shift while increasing the size of the structure.[12,13] In addition, there is an effect in the transition energy for different barrier thicknesses and Al contents in the $Al_{1-x}Ga_xN$ barrier. All these effects, i.e., growth, fabrication and optical characterisation were shown experimentally in many works.[12,14] Despite this large number of reports, there are very few simulation investigations that show the effect of electric field in such quantum structures.[15,16] Therefore, the main objective of this simulation work is to systematically study the effect of electric field in the transition energy of the QWs while varying the electric field in a particular range, the QW thickness, the composition of Al and the barrier thickness.

2. SIMULATION

Herein, we used a free simulator 1D Poisson for calculating the energy band diagram for semiconductor structures. It basically solves the 1D Poisson and Schrödinger equations self-consistently, considering the effect of quantum confinement. [17]

$$\nabla.\vec{D} = \rho \tag{1}$$

$$-\frac{\hbar}{2m^*}\Delta\psi + V = \epsilon\psi \tag{2}$$

The symbols represent: the electric displacement field ($\vec{D}$), the charge density (ρ), the reduced Planck constant ($\hbar$), effective mass (m^*), the potential function V, the wave function (ψ) with its associated energy . More details about the theory can be found elsewhere.[17,18] The band diagram of GaN/$Al_{1-x}Ga_xN$ structures is calculated using 1D Poisson (Figure 1) and the bandgap energy is found from the two band edges by taking the difference between the bottom of the conduction band and the top of the valence band. Note that the bandgap energy and the transition energy are different. In quantum structures, the Eigen electron states are above the conduction band edge and the Eigen hole states are below the valence band edges owing to the confinement effect. Transition occurs between the conduction band Eigen states to the valence band Eigen states thus the energy is higher than the bandgap energy. Nevertheless, in this study we plotted different graphs by varying different parameters utilising this simulator.

3. RESULTS AND DISCUSSION

As the wurtzite structure of GaN and related material suffers from strong built-in electric field, it has a great influence on the property of GaN/AlGaN QW. The amount of this electric field is in the range of several MV cm^{-1}.[8] Note that both in Figures 1 and 2, the Al content of the barrier is fixed at 30%, to see the effect of electric field. The Al content of the barrier is varied in Figure 3 to observe its effect on the bandgap energy. To see the effect of this large electric field, Figure 1 shows the electronic band structure of GaN QW, in which three different electric fields ranging from 0 MV cm^{-1} to 4 MV cm^{-1} are chosen.[7,8] The thickness of the well is 12 nm and the thickness of $Al_{0.7}Ga_{0.3}N$ barrier is 25 nm. In Figure 1, there is no influence of the built-in electric field on the conduction band and the valence band edges when the electric field is 0 MV cm^{-1}, as in Figure 1(a), with no evidence of band tilting observed. In contrast there is a large, shown in Figure 1(b) and larger, as in Figure 1(c), band tilting for the electric field of 2 MV cm^{-1} and 4 MV cm^{-1}, respectively. This band tilting leads to the reduction of bandgap energy as well as transition energy, which can be stated as stark shift in the transition energy. The electric field basically shifts the electron states to the lower energies and hole states to higher energies.[7] Moreover, this electric field causes the spatial separation of electrons and holes thus reduces the overlapping of their wave-function affects the oscillator strength leads to increase of radiative recombination time.[9] In the case of 4 MV cm^{-1} electric fields, the bandgap energy is found lower than the bandgap

energy of 2 MV cm^{-1} electric fields and 0 MV cm^{-1} electric fields. Therefore, as expected, the radiative recombination time for the case of 4 MV cm^{-1} electric field will be higher than the case of 2 MV cm^{-1} and 0 MV cm^{-1} electric fields.[7–9]

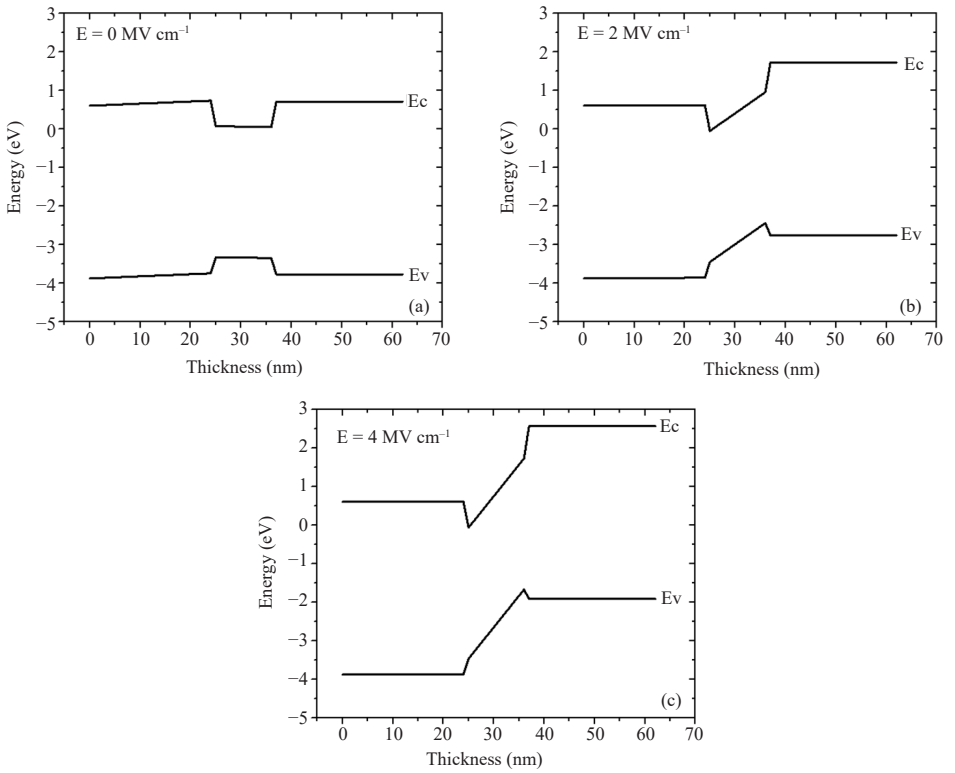

Figure 1: The electronic band structure of GaN/$Al_{1-x}Ga_xN$ (x = 0.3) QWs for (a) electric field 0 MV cm^{-1}, (b) 2 MV cm^{-1}, and (c) 4 MV cm^{-1}. The QW thickness and barrier thickness are 12 nm and 25 nm, respectively.

In Figure 2, the effect of QW thickness for different electric field is shown. For this purpose, we varied the QW thickness ranging from 3 nm to 12 nm and introduced three different electric fields. When the electric field is at 0 MV cm^{-1} we do not see any change in the bandgap energy with the thickness. The bandgap energy remains at around 3.3 eV. On the other hand, the bandgap energy reduces with the QW thickness for higher electric field such as 2 MV cm^{-1} and 4 MV cm^{-1}. The increase in QW thickness and the associated large electric field significantly reduce the bandgap energy.[12,14,18] Hence the separation of electron and hole wave function will be larger for a QW thickness of 12 nm compared to the other lower QW thickness. Accordingly, in 12 nm QW thickness the radiative recombination time will be higher than other lower QW thickness.[10]

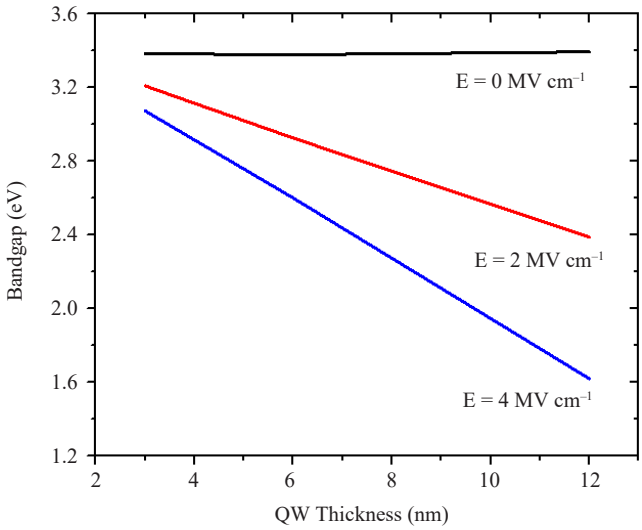

Figure 2: Effect of QW thickness on bandgap energy for different electric fields. QW thickness is varied from 3 nm to 12 nm. The $Al_{1-x}Ga_xN$ (x = 0.3) barrier is fixed at 25 nm.

Note that, the built-in electric field depends on the width of the well and barrier. However, in this study the electric field is kept at 4 MV cm^{-1} as shown in Figure 3 and Figure 4. The first reason is that the electric fields in GaN QWs are experimentally determined to be on the order of several MV cm^{-1}.[8] The second reason is to make the study simple so that the variation of other parameters can be understood.

In Figure 3, the bandgap energy is plotted as a function of barrier Al content (1-x) for different QW thickness. Here, the barrier thickness is 25 nm and electric field is fixed at 4 MV cm^{-1}. Clearly, the bandgap energy increases linearly with the Al content (1-x) for the QW thickness of 3 nm, 6 nm and 12 nm.[12,14] However, there is a disruption at 50% Al content of the barrier for 12 nm thick QW. The bandgap is negative at 30% Al content of the barrier as the conduction band edge is below the valence band edge. The simulation predicts that this phenomenon also occurs for more than 12 nm thick barrier (not shown here); however, the enhancement in the negative bandgap is less significant. Nevertheless, the blue energy shift in all cases suggests that the built-in electric field is reduced for high Al content in $Al_{1-x}Ga_xN$ barrier. This reduction of electric field is even more significant for QW thicknesses 6 nm and 12 nm, as in the graph the slope of 6 nm and 12 nm thick QW are higher than the 3 nm thick QW.

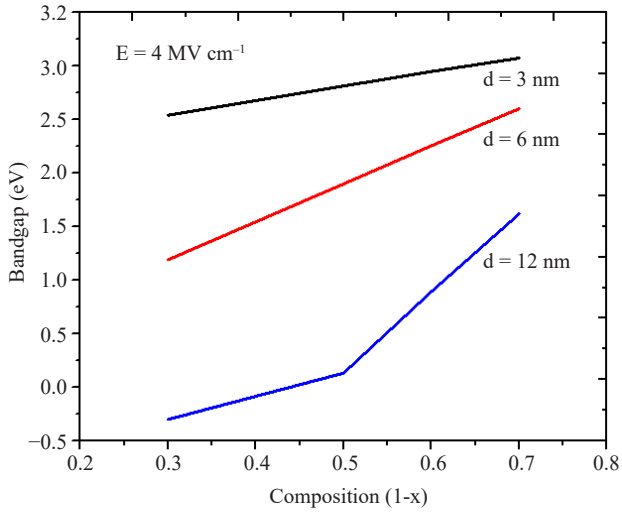

Figure 3: The effect of Al content (1-x) on the bandgap energy for different QW thickness. The barrier is 25 nm thick.

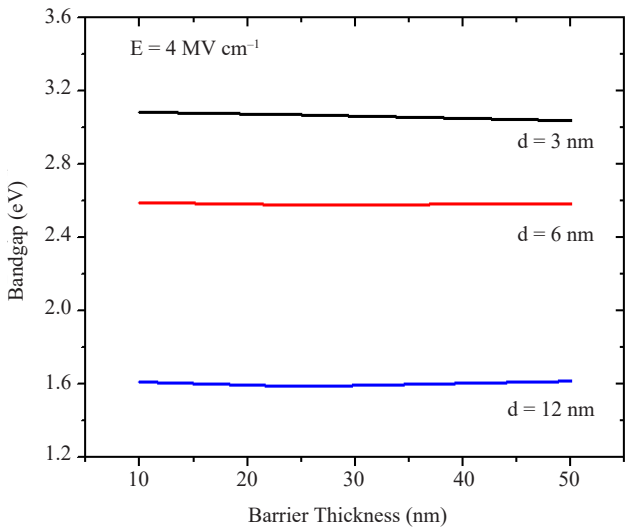

Figure 4: The bandgap energy as a function of $Al_{1-x}Ga_xN$ barrier thickness. The electric field is fixed at 4 MV cm^{-1}.

Nevertheless, the blue shifted bandgap energy with Al content of $Al_{1-x}Ga_xN$ barrier in all cases indicates that there is an enhancement in the overlapping between the electron and hole wave functions. This is true for different QW thickness studied here. Besides, if any specific Al content of the $Al_{1-x}Ga_xN$ barrier is considered then the radiative recombination time will increase for higher QW thickness.

Figure 4 shows the effect of $Al_{1-x}Ga_xN$ barrier thickness on the bandgap energy for different QW thicknesses, while the electric field is kept at 4 MV cm^{-1}. Here, the barrier thickness is varied from 10 nm to 50 nm.[12,14] It is evident that, within this barrier thickness range the bandgap energy slightly decreases only for the 3 nm thick QW. On the other hand, for QWs with the thicknesses of 6 nm and 12 nm, the bandgap energy shows almost a flat line. Therefore, it indicates that the barrier thickness is independent of the bandgap energy for a fixed electric field. It suggests that the considered barrier thicknesses have no effect on the confinement of the electrons in the conduction band and holes in the valence band.

4. CONCLUSION

In summary, we investigated the effect of electric field on the electronic band structure of $GaN/Al_{1-x}Ga_xN$ QW. It shows that higher electric fields result in more tilt in the band edge leading to lower bandgap energy. This bandgap energy reduces with the QW thickness for electric fields in the order of few MV cm^{-1}. Moreover, we observed that the bandgap energy increases with the Al content (1-x) for different QW thicknesses. In addition, we studied the effect of $Al_{1-x}Ga_xN$ barrier thickness on the bandgap energy. It is found that for a fixed electric field of 4 MV cm^{-1}, the barrier thickness is independent of the bandgap energy.

5. ACKNOWLEDGEMENTS

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