

Effect of Spontaneous and Piezoelectric Polarization on the Optical Properties of AlGa_N/Ga_N Quantum Well

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ABSTRACT: The properties of Group III- nitrides are that they have a large and direct band gap structures. Due to these properties, there is a large lattice mismatch among the nitride heterostructures. The large lattice mismatch results in strain. Polarization occurs in the heterostructure due to the strain which in turn is a cause of the generation of internal electric field. Internal electric field creates a transition energy, that is photoluminescence. This generation of transition energy for AlGa_N/Ga_N quantum well and necessary calculations are discussed in this paper. In this paper finite difference method (FDM) is used for calculating transition energy.

KEYWORDS: Quantum well (QW), finite difference method (FDM).

I. INTRODUCTION

GaN based quantum wells have attracted much interest in the last few years since they have become the key material in commercial fabrication of longtime LED's and laser diodes. GaN has a large peak electron velocity, larger saturation velocity and thermal stability making it suitable to be used as a channel material in microwave power devices [1]. Thus we have considered strained AlGa_N/Ga_N quantum well here, since it has been a subject of intense recent investigation and have emerged as attractive candidate for high voltage, high power operation and microwave frequency [2]. The lattice mismatch of the epitaxial layer of AlGa_N with Ga_N is 3.8%. The higher lattice mismatch percentage for AlGa_N/Ga_N quantum well leads to high strain. Another peculiarity results from the polar axis of the wurtzite crystal structure and the strong polarity of III-N bindings. All group-III nitrides in the wurtzite phase have a strong spontaneous macroscopic polarization and large piezoelectric coefficients. This has been found from *ab initio* calculations [3, 4, 5]. The abrupt variation of polarization at the surfaces and interfaces gives rise to large polarization sheet charges that in turn create internal electric fields of the order of MV/cm. In this paper, we calculate the internal electric field which is generated due to both spontaneous polarizations and piezoelectric polarizations and also calculate the one to one transition energies of AlGa_N/Ga_N quantum well by finite difference method (FDM).

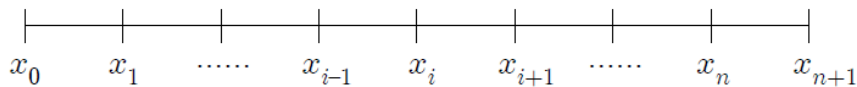
II. THEORETICAL DETAILS

According to quantum mechanics, the state of the electron moving in one dimensional space within a potential $V(x)$ can be described by a time-independent Schrodinger's Equation:

$$\frac{-\hbar^2}{2m} \frac{d^2\Psi}{dx^2} + V(x)\Psi(x) = E\Psi(x) \quad (1)$$

where, x is the space position, function $\psi(x)$ is called the wave function of the electron, E is a scalar, represent energy of electron. According to quantum mechanics, the energy level of electron is discretized. The lowest energy state E_0

represent the ground state of electron, then higher energy level E_1, E_2, E_3, \dots , represent the first, second, third, ... excited states. There is a wavefunction $\psi_i(x)$ corresponding to each energy eigenvalues E_i , so wavefunction $\psi_i(x)$ is also called eigenfunction of Schrodinger equation. Given one specific potential $V(x)$, our task is to find the energy eigenvalues E_i and their corresponding eigenfunctions $\psi_i(x)$. Several numerical methods can be applied to compute the eigenvalues and eigenfunctions by solving Schrodinger equation. In this paper, a finite difference method (FDM) is used. The first step is to discretize the x axis by $x_i = \Delta x * i, i = 0, 1, 2, \dots, n + 1$ as shown



Then discretize the differential equation to:

$$-t_0 \frac{\psi_{i+1} + \psi_{i-1} - 2\psi_i}{\Delta x^2} + V(x)\psi_i = E\psi_i \tag{2}$$

where
$$t_0 = \frac{\hbar^2}{2ma^2} \tag{3}$$

\hbar^2 is the planks constant, m is the effective mass and a is $x_1 - x_0$, the boundary conditions are $\psi_0 = 0, \psi_{n+1} = 0$

$\frac{\psi_{i+1} + \psi_{i-1} - 2\psi_i}{\Delta x^2}$ can be written in the form of a tridiagonal matrix

$$E \begin{bmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_n \\ \vdots \\ \psi_N \end{bmatrix} = t_0 \begin{bmatrix} 2 & -1 & 0 & 0 & 0 \\ -1 & 2 & \ddots & 0 & 0 \\ 0 & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & \ddots & 2 & -1 \\ 0 & 0 & 0 & -1 & 2 \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_n \\ \vdots \\ \psi_N \end{bmatrix} \tag{4}$$

TRI-DIAGONAL MATRIX

$V(x)$ the profile of the trapezoidal AlGa_N/Ga_N quantum well, which is measured for both conduction band and valence band profile. To calculate the profile, we need the values of spontaneous and piezoelectric polarization, the value of electric field for each Al mole fraction, the relative and absolute permittivity and the well width.

The total polarization is given by

$$P = P_{sp} + P_{pz} \tag{5}$$

where P_{sp} is spontaneous polarization and P_{pz} is piezoelectric polarization

$$P_{spAlxGa1-xN} = P_{sp}^{AlN} x + P_{sp}^{GaN} (1-x) \tag{6}$$

$$P_{pz}^{AlGaN} = 2 * ((a^{GaN} - a^{AlGaN}) / a^{AlGaN}) * (e_{31} - (e_{33} * (c_{13} / c_{33}))) \tag{7}$$

The built in electric field is given by

$$F = -\{ (P_{sp}^{AlGaN} + P_{pz}^{AlGaN}) - (P_{sp}^{GaN} + P_{pz}^{GaN}) \} / (8.854 * 10^{12} * \text{dielectric constant}^{AlGaN}) \tag{8}$$

$V(x)$ is the diagonal matrix representation of the trapezoidal quantum well profile for which

$$V(x) = \begin{cases} -V_{e(h)} + eFx, & -\frac{L}{2} \leq x \leq \frac{L}{2} \\ eFx, & -\frac{3L}{2} \leq x \leq -\frac{L}{2} \quad \text{and} \quad \frac{L}{2} \leq x \leq \frac{3L}{2} \end{cases} \tag{9}$$

Where e is the charge of electron, a is $x_1 - x_0$ and F is the built in electric field.

The total Hamiltonian is given by

$$H = \begin{bmatrix} 2t_0 + V(x^1) & -t_0 & 0 & 0 \\ -t_0 & 2t_0 + V(x^2) & \ddots & 0 \\ 0 & \ddots & \ddots & 0 \\ 0 & 0 & 0 & 2t_0 + V(x_n) \end{bmatrix} \quad (10)$$

Now the total value for the transition energy can be determined by the following equation

$$E_{transition} = E_g^{AlGaIn} + E^l_{conduction} + E^l_{valence} \quad (11)$$

TABLE-1

Wurtzite	GaN	InN	AlN	InGaIn	AlGaIn
Bulk bandgap energy (eV)	3.4	0.7	6.2	3.4(1-x)+0.7x-bx(1-x) (free-standing)	3.4(1-x)+6.2x-bx(1-x) (free-standing)
A ₀ (Å)	3.189	3.545	3.112	Vegard's law	Vegard's law
c ₀ (Å)	5.185	0.5703	4.982		
e ₃₃ (C/m ²)	0.73	0.97	1.55		
e ₃₁ (C/m ²)	-0.49	-0.57	-0.58		
c ₁₃ (Gpa)	106	92	108		
c ₃₃ (Gpa)	398	224	373		
Relative permittivity ε _r	10.4	14.6	9		
m _e /m ₀	0.18	0.14	0.32		
m _h /m ₀	1.61	1.68	0.30		
Band offsets ratio	0.61/0.39				
P ^{SP}	-0.042	-0.034	-0.090		

III. RESULTS & DISCUSSIONS

Figure 1(a) shows the variation of Al concentration with the spontaneous polarization for AlGaIn/GaN quantum well. The graph shows that spontaneous polarization varies inversely with the Al concentration. Figure 1(b) shows the variation of piezoelectric polarization for AlGaIn/GaN quantum well with Al concentration. Here we see that the piezoelectric polarization is inversely proportional to the Al concentration

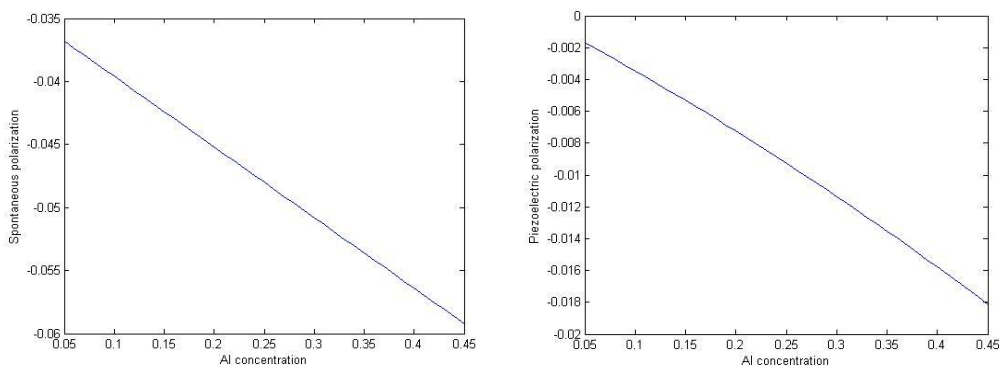


Fig 1 (a)The variation of Al mole fraction with spontaneous Polarization (b) Variation of Al mole fraction with Piezoelectric polarization

Figure 2 shows the variation of Al mole fraction of the material AlGa_N/Ga_N with respect to the built in electric field in MV/m. Here we can observe that the built in electric field for AlGa_N/Ga_N quantum well increases almost linearly with the Al mole fraction.

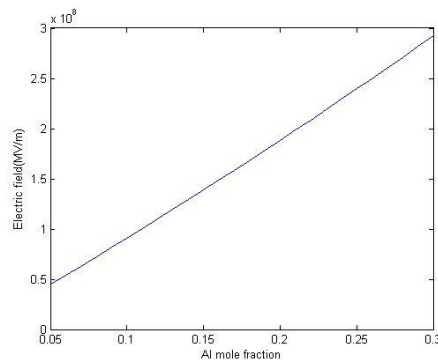


Fig 2: Variation of Al mole fraction with built in electric field

Figure 3(a) shows the variation of Al concentration with the transition energy of AlGa_N/Ga_N quantum well. Here we see that the transition energy gradually decreases with the increase in Al concentration. Figure 3(b) shows the variation of Transition energy with the well width for Al concentration 0.2. Here we see the transition energy gradually decreases with the increase in well width.

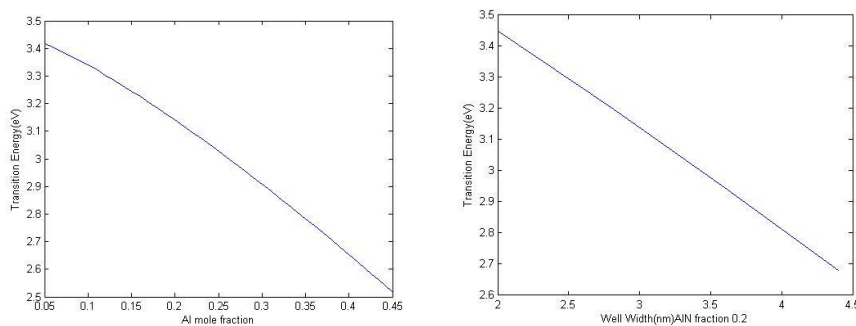


Fig 3(a): Variation of Al mole fraction with transition energy (b) Variation of well width with transition energy

IV. CONCLUSION

In conclusions, we have shown that strain increases due to change in Al concentration and also shown that the internal electric field generated due spontaneous and piezoelectric polarization. Finally we observe that the optical properties of AlGa_N/Ga_N quantum well are strongly affected by the internal electric field originated due to spontaneous and piezoelectric polarization.

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