Strain Effects on Band Structure of Wurtzite InGaN/GaN Quantum Well on Si Substrate

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Abstract Heteroepitaxial crystal growth of InGaN/GaN Quantum Well (QW) on Si substrate is necessary for the development of visible and ultraviolet (UV) Light Emitting Diodes (LEDs). In this work we accumulate the efforts that have been made to focus the analysis of strain effects on the band structure of GaN quantum well systems on Si substrate due to its potential application. We limit this investigation on the effect of pseudomorphic GaN quantum wells on Si substrate grown at different GaN planes. It is observed that the deformation potential constants and anisotropic strain separate Heavy Hole (HH) and Light Hole (LH) band and eventually making LH the top most bands.

1. Introduction

The development of LED devices on Si substrate using InGaN/GaN is quite challenging because of significant lattice mismatch (almost 16%, leading to strain in the GaN layers) and thermal mismatch (approximately 54%) between Si and GaN. Presently the InGaN/GaN QW Light Emitting Diodes are fabricated on SiC, Sapphire (α-Al2O3) or Si substrate. The GaN, InN and their ternary alloy materials have a wurtzite crystal structure and a direct energy bandgap. At room temperature the band gap of GaN and InN are 3.44eV and 1.89eV respectively [1]. The band gap of the ternary alloy InxGa1-xN can be interpolated using Vegard’s law [2]. This band gap depends on the mole fraction of In. In that case a bowing parameter is also taken into account. GaN/InGaN based blue and green light emitting diodes (LED) are very important for shorter wavelength application [3-5]. The optical properties of the LED devices depend significantly on the epi-layer quality. Different types of substrates are used for growing InGaN/GaN quantum well layer such as 6H-SiC, Sapphire, and Si. Our main focus is to investigate devices on Si substrate because of its obvious benefits [6]. In the pseudomorphic growth, strain is generated in the epitaxial layers. This strain modifies the band structure [7-10]. We have investigated this phenomenon.

2. Effect of strain on valance band spectra in pseudomorphic InGaN/GaN quantum wells

The idea of quantum well first took shape when Esaki and Tsu [11, 12] suggested in 1969 that a heterostructure sandwich of ultrathin layer of two semiconductors with different band gaps should exhibit some novel useful properties. The band-edge potential varies from layer to layer due to different band gaps and a periodically varying potential is produced in the structure for layer thickness of the order of few nano meters. The band structure of the quantum well is modified by this strain. The effect of strain on the band structure of semiconductor was first presented by Bir and Pikus [13]. The unstrained lattice
vectors \( \mathbf{x}_i \) and the strained lattice vectors \( \mathbf{x}_i' \) are related through the relation 

\[ x_i' = x_i + \sum_j \epsilon_{ij} x_j, \]

where \( \epsilon_{ij} \) denote the strain tensor components. A model for the electronic band structure of wurtzite strained quantum well was presented in [14] by introducing strain effect on \( k.p \) band structure. This theoretical model provides a foundation of wurtzite-strained quantum well LED. The band edge energy of the conduction band \( E_c \), the HH, the LH, and the CH bands are shown in Fig.1.

The same band structure of strained semiconductor was modified with the introduction of spin-orbit split-off bands coupling by C.Y.P. Chao et al. [15]. As a result the \([6 \times 6]\) Hamiltonian at the band edge at \( K=0 \), is takes a new form. The most important results are obtained from the series expansion of \( E \) up to the second order of \( K \) near the band edges given by:

\[
E_{HH}(k) \approx E_{HH}(0) - \left( \frac{\hbar^2}{2m_0} \right) \left[ (\gamma_1 + \gamma_2)K_t^2 + (\gamma_1 - 2\gamma_2)K_z^2 \right],
\]

\[
E_{LH}(k) \approx E_{LH}(0) - \left( \frac{\hbar^2}{2m_0} \right) \left[ (\gamma_1 - f_+\gamma_2)K_t^2 + (\gamma_1 + 2f_+\gamma_2)K_z^2 \right],
\]

\[
E_{SO}(k) \approx E_{SO}(0) - \left( \frac{\hbar^2}{2m_0} \right) \left[ (\gamma_1 - f_-\gamma_2)K_t^2 + (\gamma_1 + 2f_-\gamma_2)K_z^2 \right],
\]

where \( f_+ \) and \( f_- \) are dimensionless, strain-dependent factors.

A further improvisation on this theoretical study based on the RSP Hamiltonian uses Envelop function analysis which successfully explains the origin of piezoelectric effects [16]. The piezoelectric polarization \( P_{piezo} \) is generally formulated using Vegards’s interpolation formula [17]. For valance band they have used \([6 \times 6]\) Hamiltonian in block diagonal forms [18]. Fig. 2 shows the valance sub band dispersion spectrum of \( \text{In}_{0.16}\text{Ga}_{0.84}\text{N}/\text{GaN} \) QW structure caused by internal polarization field. In this case the blue energy shift of all states is caused by the indium surface segregation effect. Here the energy shift is 20meV for the valence band amounting to a total blue shift of 70mev. The effects of strain on the valence band structure of \((1\bar{1}22)\) semipolar InGaN grown on GaN were analyzed by \( k.p \) method also by Qimin Yan et al [20] which showed that the anisotropic strain the c-plane and shear strain are the most important factors for decoding the ordering of the two top most valence bands. The shear strain deformation potential \( D_6 \) is often calculated for GaN and InN using density functional theory with the Heyd – Scuseria – Emzerhof hybrid function. [21]
Under shear strain, the $E_2$ band goes up may switch order with the $E_1$ band [20]. It also gives a measure of the Energy separation $\Delta E_{23}$ between valence bands $E_2$ and $E_3$. It is seen that InGaN/GaN MQWs structure suffers from anisotropic in-plane compressive strain, breaking the original valence band states [22]. The peak energy shifts results from the splitting valence sub-bands that rises with increase of in-plane strain [23]. Conversely reduction of strain leads to the reduction of the polarization ratio [24, 25]. Due to strain, the VB states are strongly modified affecting both the energies as well as the polarization selection rules for the transitions. Hamiltonian for the strain dependence of the VB can be modeled by [26] yielding three distinct VB maxima with energies $E_j^{\nu}$. The parameter values thus obtained are $\alpha_\perp = \alpha_\parallel = -44.5\, eV$, $D_1 = -41.4\, eV$, $D_2 = -33.3\, eV$, $D_4 = -4.1\, eV$, and $D_5 = -4.7\, eV$. The resulting inter band hydrostatic deformation potentials are $\alpha - D_1 = -3.1\, eV$ and $\alpha - D_2 = -11.2\, eV$. The calculation of reference [25] gave slightly modified values of deformation potential at $D_3 = 9.4\, eV$, and $D_4 = -4.7\, eV$. The diagonalization of the traditional $[6\times6]$ VB Hamiltonian was reduced to give three distinct sub-band dispersion relations, where each sub-band is a Kramers degenerate pair [27]. At $\Gamma$ point, where $k=0$, the VB Hamiltonian is automatically blocked diagonalized as:

$$H(k=0, \varepsilon) = \begin{pmatrix} H^U & 0 \\ 0 & H^L \end{pmatrix}, \text{ where } H^U = \begin{bmatrix} F_0 & -K_0^* & 0 \\ -K_0 & G_0 & \sqrt{2}\Delta_3 \\ 0 & \sqrt{2}\Delta_3 & \lambda_0 \end{bmatrix}$$

Where, $H^L$ is the complex conjugate of $H^U$. References [28] and [29] further reformed the Hamiltonians and their interband optical matrix elements for three important crystal orientation; namely c-plane, m-plane, and a-plane by using multiband effective mass theory. It is to be noted that strain in any form has a degrading effect on the performance and as a preventive measure usage of pre-strained layer has been suggested for partial relaxation resulting in improvement of the quantum efficiencies of the LED [30].

3. Conclusion

In summary we have analyzed the various theories for band structure modification of InGaN/GaN quantum wells due to strain. It is seen that generation of the piezoelectric field is the primary cause for alteration of valance band structure in the quantum well.

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