

Optical analysis of non-polar, m-plane GaN/AlGaIn quantum cascade structures

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Abstract— A quantum cascade structure (QCS) for the mid-infrared (IR) photon detection has been designed using non-polar, m-plane III-nitride material system. The effect of temperature and active layer doping on the absorption coefficient has been studied theoretically for the designed QCS.

I. INTRODUCTION

A special class of intersubband (ISB) devices is quantum cascade (QC) devices that use the concept of cascaded transport of carriers through a quantum cascade structure (QCS) for the device operation. A lot of research is going on to extend the QC device technology in the whole IR spectral region with remarkable performance characteristics. A notable approach is the use of different material systems for designing of the QC device in order to improve their performances. Non-polar III-nitrides are the next in the list and it is expected to get more improved device performance with much larger wavelength coverage in the IR spectral range with larger design space compared to polar III-nitrides. Non-polar nitrides are free from internal polarization fields while they maintain the advantages of III-nitrides.

In this paper, we have designed a three well QCS applicable for mid-IR detection of radiations. Carrier energies and wave functions associated with the structure are obtained by solving the coupled Schrödinger-Poisson equation for the structure self-consistently using finite difference method. Conduction band nonparabolicity has been considered in the process of band solution through the energy dependent effective masses of electrons for accurate results. Temperature dependent material parameters have been included to get the proper temperature response of the structure. Our simulation results have been compared with many experimental results available in literature. A very close matching of our results with experimental results has been observed. Further, we have obtained the absorption coefficient for the proposed structure and effects of temperature, active layer doping have been examined.

II. THEORETICAL FORMULATION

In order to obtain the optical properties of nonpolar, m-plane III-nitride QCSs, it is required to attain the carrier energies and wave functions associated with the structure accurately. Solution of the Schrödinger equation provides necessary information regarding energies and wave functions. The one dimensional Schrödinger equation for an electron in effective mass approximation is given as

$$-\frac{\hbar^2}{2} \frac{d}{dz} \left(\frac{1}{m^*(E, z)} \frac{d\psi(z)}{dz} \right) + V(z)\psi(z) = E\psi(z), \quad (1)$$

where $V(z)$ is the total potential energy [1] met by an electron when in the conduction band. The term $m^*(E, z)$ is the electron effective mass which varies spatially along growth direction (z) due to hetero-epitaxial growth of III-nitride QCS layers and depends on the energy position of the subbands in QCS. The energy dependence of the electron effective mass arises because of conduction band nonparabolicity effect. The energy dependent electron effective mass can be obtained as [2]

$$m^*(E, z) = m^*(z)[1 + \alpha(E - V)], \quad (2)$$

where $\alpha = (1 - m^*(z)/m_0)^2 / E_g(x, T)$ is the nonparabolicity parameter with free electron mass m_0 and $m^*(z)$ is the electron effective mass under parabolic band approximation. The temperature dependent bandgap of $\text{Al}_x\text{Ga}_{1-x}\text{N}$ material can be obtained using Varshni relation [1].

The conduction band offset energy for GaN well and $\text{Al}_x\text{Ga}_{1-x}\text{N}$ barrier structure is given as

$$\Delta E_C = 0.61 \times [E_g(\text{Al}_x\text{Ga}_{1-x}\text{N}) - E_g(\text{GaN})]. \quad (3)$$

The fraction for the conduction band offset is taken as 0.61 after inspection which gives experimental accuracy for the band solution and closely agrees with the extracted band offset ratio by Hurni *et al.* [3] based on experimental observations.

To get proper band solution for the m-plane nonpolar III-nitride QCS, self-consistent solution of coupled Schrödinger-Poisson equation with periodic boundary condition has been carried out following our previous work for polar III-nitride QCSs [1]. The only difference in the band solution will be the polarization field contribution in the Poisson equation, which has to be taken as zero as the non-polar, m-plane III-nitrides are free from internal polarization fields.

The intersubband absorption coefficient for a QCS is given as [1]

$$\alpha_{abs}^{if} = \frac{n_{if} e^2 \hbar}{2\epsilon_0 c n_{ref} m^*} f_{if} \frac{\gamma}{(E_f - E_i - \hbar\omega)^2 + \gamma^2}, \quad (4)$$

All the terms in the equation carry their usual significances.

III. RESULTS AND DISCUSSION

We have designed a GaN/Al_{0.6}Ga_{0.4}N QCS for mid-IR (~ 4 μm) detection purpose. The band diagram, energies and corresponding wave functions are plotted in Fig. 1.

To validate our band solution results, we have run our Schrödinger-Poisson solver for the quantum well (QW) structures reported in literatures and compared results with our results and listed in Table I. It is observed that results obtained

considering band nonparabolicity gives more exact results in terms of experimental accuracy.

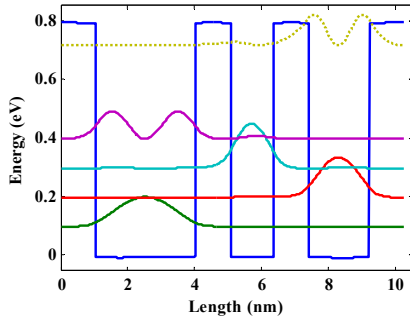


Fig. 1. The energy band diagram of a single period of m-plane III-nitride QCS. The consecutive layer thicknesses (in nm) of a QCS period are given as follows: **1.04/2.99/1.04/1.3/1.04/1.82/1.04**. Al_{0.6}Ga_{0.4}N barriers are represented in a bold font. The QW layer underlined is the active well which is intentionally doped to populate the ground energy level of the active well.

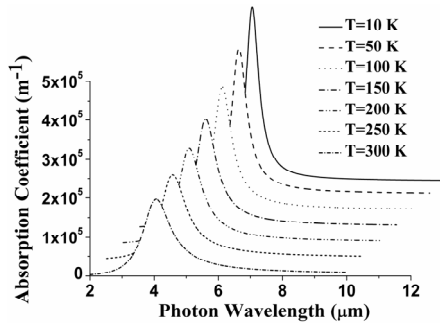


Fig. 2. Absorption coefficient of the QCS at different temperatures.

Next, we have obtained the absorption coefficient of the QCS for different temperatures and plotted against photon wavelength for a particular doping density ($7 \times 10^{24} \text{ m}^{-3}$) as shown in Fig. 2. The decrease of the absorption coefficient with temperature is mainly due to the decrease of the conduction band offset, increase of the thermal population at higher absorption state and absorption linewidth broadening because of temperature dependent scattering processes. The red-shift of the absorption wavelength is mainly due to the temperature dependent conduction band edge shift in these non-polar III-nitride materials which effectively decreases the conduction band offset; hence the absorption energy. It is worth mentioning that the temperature dependent red shift of the absorption wavelength for m-plane III-nitride QCS is significantly small of the order of 0.8 meV for a temperature variation from 10 K to 300 K. This result implies that, stable wavelength detection can be achieved for a wide range of temperatures using m-plane III-nitride QCSs.

The results for different active layer doping densities at a fixed temperature ($T=300 \text{ K}$) have been plotted in Fig. 3 with respect to photon wavelength. It is observed that absorption coefficient increases with the increase in doping density which is mainly because of increase in carrier population in the lower absorption state. An obvious blue shift of the absorption wavelength (19.5 meV energy shift for the doping density variation from $2.3 \times 10^{24} \text{ m}^{-3}$ to $2.1 \times 10^{25} \text{ m}^{-3}$) has been observed. The blue shift in the absorption wavelength is ascribed mainly by many body effects. This result agrees with the experimental result observed for m-plane III-nitride multiple QWs by Kotani *et al.* [4] where an energy shift of 29.5 meV is obtained for the doping density variation from $2.3 \times 10^{24} \text{ m}^{-3}$ to $2.1 \times 10^{25} \text{ m}^{-3}$.

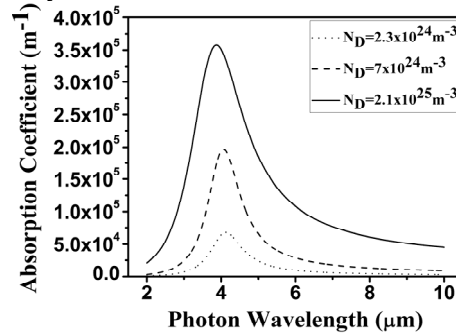


Fig. 3. Absorption coefficient of the QCS for different active layer doping densities.

IV. CONCLUSION

In this paper, nonpolar, m-plane III-nitride QCS designed for the mid-IR photon detection has been analyzed theoretically. The effect of temperature, doping and electric field on the absorption coefficient has been examined. A better conformity of the theoretical results with the experimental results has been achieved.

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TABLE I. COMPARISON OF THE ABSORPTION PEAK ENERGY OBTAINED IN THIS PAPER WITH THE RESULT REPORTED IN LITERATURE FOR DIFFERENT M-PLANE III-NITRIDE QW STRUCTURES.

Reference	GaN well width (nm)	AlGaIn barrier width (nm)	Al mole fraction in the barrier	Doping density (cm ⁻³)	T (K)	Absorption peak energy (meV)			
						(from the reference)		Simulation (our results)	
						Experimental	simulation	With parabolic approximation	With nonparabolicity correction
Ref. [4]	2.85	3.2	0.485	7×10^{18}	8.4	287.9	Not available	298.8	286.6
					300	285.3	285	298.2	285.7
Ref. [5]	2.7	3	0.5	7×10^{18}	300	295	286	322.7	308.3
	3.3				256	233	250.5	241.4	