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Cathodoluminescence Calculation of AlGaN/GaN Quantum-Wells by MonteCarlo Model: Effect of Compositional and Temperature

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ABSTRACT

In this paper, a AlGaN/GaN multi-quantum wells (MQWs) with $Al_xGa_{1-x}N$ barriers and GaN quantum wells have been studied using Monte Carlo calculations and cathodoluminescence (CL) technique, in this study we demonstrate the influence of important parameters such as Al mole content (x) and temperature (T) in AlGaN/GaN. The cathodoluminescence signal CL is calculated in AlGaN/GaN taking into account compositional, temperature and confinement phenomenon of electrons within the quantum well of GaN.

Keywords: Monte Carlo, Cathodoluminescence, AlGaN/GaN, quantum well.

INTRODUCTION

The III–V nitride materials are very important due to their wide band gap [1], in addition Monte Carlo methods are widely used for complex physical problems. This numerical method can be used to simulate electron trajectories. Cathodoluminescence is a very useful tool for the characterization of low-dimensional structures. In this paper, cathodoluminescence model of AlGaN/GaN multi quantum wells has been studied by Monte Carlo calculation method to describe the interaction of electron beam with $Al_xGa_{1-x}N$/GaN nanostructure. This model takes into account the x mole content of aluminium and temperature variation. The radiative recombination of electron-hole pairs is collected as a light (CL signal).

MODEL

The electron hole pair creation energy is given by [2]:

$$E(e-h) \approx 3Eg \quad (1)$$

Eg: Band gap energy, the step distance S is written as :

$$s = -\lambda \ln(R) \quad (2)$$

Where R is a random number between 0 and 1. The mean free path λ can be obtained from the total scattering cross section as :

$$\lambda = \frac{A}{N_A \rho \sigma} \quad (3)$$

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Where A is the atomic weight (83.73 g for GaN), N_A is the Avogadro's number, ρ is the density of the material (ρ=3.5 g/Cm^3). The total relativistic Rutherford scattering cross section is given by:

$$\sigma = 5.21\times10^{-21}.\frac{Z^2}{E_e^2}.\frac{4\pi}{\delta(1+\delta)}.\left(\frac{E_e+m_0c^2}{E_e+2m_0c^2}\right)^2 \quad (4)$$

Where *Z* is the atomic number of the scattering atom (Z=19 for GaN), E_e is the energy of electron in keV, *C* is the speed of light, m_0 is the mass of electron, and δ is a screening parameter.

The band gap of $Al_xGa_{1-x}N$ has been described by [3]:

$$E_g(x,T) = E_g(x,0) - \frac{\alpha(x)T^2}{\beta(x)+T} \quad (5)$$

The measured compositional dependence of α and β in $Al_xGa_{1-x}N$ alloys for 0 ≤ x ≤ 1 is based on experimental data,

The CL signal (I_{CL}) is given by [4]:

$$I_{CL} \propto \int_0^{\infty} \frac{\Delta n(y)}{\tau_n} \exp(-\alpha' y)dy \quad (6)$$

RESULTS AND DISCUSSIONS

The calculated CL signal of sample is presented in Fig. 1 for $Al_{0.25}Ga_{0.75}N$/GaN at 300 K, the CL intensity presentes a maximum at quantum wells regions. A good correlation between our calcul and other result [5], we can calculete the minority carrier diffusion length L_d of $Al_{0.25}Ga_{0.75}N$/GaN/ $Al_{0.25}Ga_{0.75}N$ quantum well using $I_{QW} \sim I_{max}*\exp(-x/L_d)$ [5], CL measurements are fitted by Monte Carlo curve with L_d of *23* nm, this value is comparable to that of As et al[5] which was 20 nm.

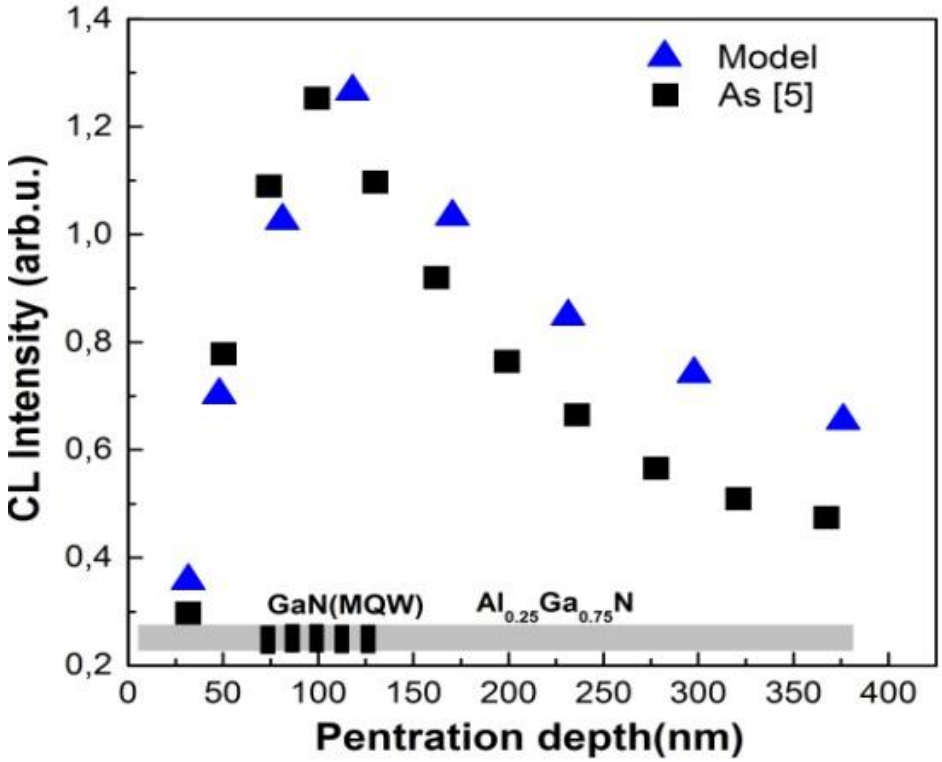

Fig. 1. Cathodoluminescence signal: comparison between our calculation model and other experimental model [5]

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CONCLUSIONS

In summary, we have calculated the signal CL of $Al_xGa_{1-x}N$/GaN nanostructure. Cathodoluminescence spectra as a function of x mole fraction and temperature was calculated in multi-quantum wells. A comparative fitting between experimental and our simulated CL signal in the case of GaN/AlGaN sample permitted a validation of our model. The diffusion length of AlGaN/GaN/AlGaN has been calculated.

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