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Monte Carlo model to study $Al_xGa_{1-x}N$ nanostructure under an electron beam. Influence of aluminum mole fraction

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Abstract
In the present paper, a Monte Carlo calculation model of $Al_xGa_{1-x}N$ nanostructure is presented in order to describe the influence of different parameters such as the accelerating energy and primary current of electron beam as well as the influence of aluminum mole fraction. The carrier excess generated during the collision of the incident electron with the atoms of the material (random walk) is calculated as a function of depth. The radiative recombination of electron hole pairs can be collected as a light (CL signal). Numerical results obtained are compared with experimental data.
Keywords: Gallium nitride, Monte Carlo, Cathodoluminescence, nanostructure, quantum well.

1. Introduction

In the last few years the technology of group III nitride epitaxy has shown great progress on modern materials and electronic devices as well as on high electron mobility transistors (HEMTs), Light emitting diodes (LED) and photovoltaic solar cell, etc [1,11].
Cathodoluminescence (CL) has been used with success in studying luminescence properties of semiconductors[6-8]. Cathodoluminescence (CL) simulation was carried out to study the heter structure of GaAs[10].
Light emitted from a specimen in response to electron-beam irradiation. The electrons and the holes recombine radiatively[13].
The Al mole fraction is a critical parameter which determines the emission wavelength in AlGaN light-emitting diodes [11,12].

2. Model

2.1 Electron-Matter Interaction

The electron-matter interaction during SEM analysis may result in a range of effects on incident electrons, which can be divided into two primary types of electron scattering: elastic and inelastic [2]. The e-h pair produced during the random walk process of the incident electrons within the sample. The simulation was performed with the following steps: (1) defining numerous random pathways ***s*** of the incident electrons in the sample (2) dividing the sample into several zones; (3) calculation of carrier excess Δn (e-h pair) within each zone based on Monte Carlo method (random walk) taking into account the conditions of the incident electron beam (e.g., accelerating voltage E_0, primary current I_0). The radiative recombination of carrier excess results cathodoluminescence signal. More detailed calculation procedures and explanations are available in Aouati *et al.* [9].

2.2 Penetration depth

The penetration depth of an incident electron can be given by:

$$R_e(\mu m) = \left(\frac{0.0276.A}{\rho.Z^{0.889}}\right).E_0^{1.75} \quad [3]$$

$$R_e(\mu m) = \left(\frac{0.0398}{\rho}\right).E_0^{1.7} \quad [4]$$

$$R_e(\mu m) = \left(\frac{25.6}{\rho}\right).\left(\frac{E_0}{30}\right)^{1.7} \quad [5]$$

Where ρ is the density of material, Z is the atomic number, A is atomic mass and Eo is the accelerating energy
But in our model, the penetration depth is calculated by a numerical method based on the random walk [9].

2.3 Cathodoluminescence signal (I_{CL})

The cathodoluminescence signal I_{CL} can be calculated by integration of minority carrier excess taking into account the absorption phenomenon:

$$I_{CL} \propto \int_0^{\infty} \Delta n\,(z) e^{(-\alpha Z)} dz$$

Where Δn is the minority carrier excess (for a p-type semiconductor), α is the absorption coefficient.

In our case, the integral becomes summation because the numerical calculation procedure:

$$I_{CL} = \sum_{i=1}^{n} \Delta n_i e^{-\alpha Z_i}$$

$$= \Delta n_1 e^{-\alpha Z_1} + \Delta n_2 e^{-\alpha Z_2} + \cdots + \Delta n_n e^{-\alpha Z_n}$$

$$= CL_1 + CL_2 + \cdots + CL_n$$

Where Δn_i is the minority carrier excess inside the zone i after the random collisions.

Table 1. Some bulk material parameters for GaN and $Al_xGa_{1-x}N$ used in our calculation. [14]

Parameter	GaN	$Al_xGa_{1-x}N$
Crystal density *g (g/cm³)*	*6.15*	*6.15-2.92x*
Energy band gap *Eg (eV)*	*3.43*	*x^2-2.43x+3.43*

3. Results and conclusion

The first main result of this work is

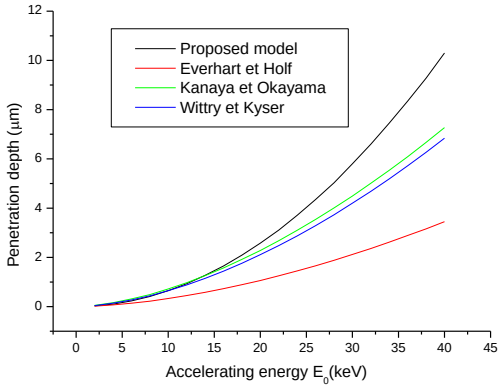

Fig.1. Penetration depth of electrons in GaN as a function of accelerating energy

The maximum electron depth is proportional to the accelerating energy.

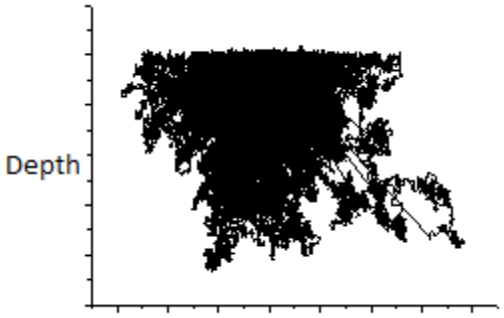

Fig.2. Monte Carlo simulations of the penetrated electrons paths into GaN

Fig.2. shows 100 simulated electron trajectories for a 20-keV electron beam.

The Al composition of $Al_xGa_{1-x}N$ layers was estimated by assuming the Vegard's law. The band gap of ternary compound depends on composition fraction X is given by:

$Eg_{AlGaN}(x) = x^2 - 2.43x + 3.43$ eV (hexagonal) [14].

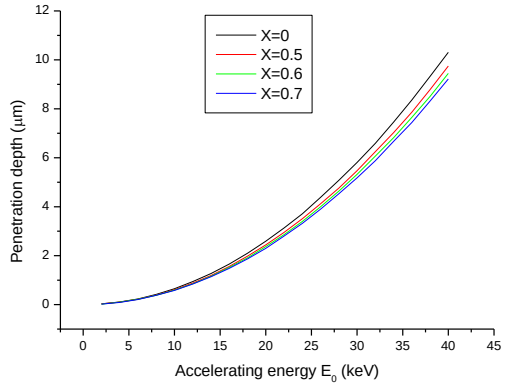

Fig.3. Penetration depth of electrons in AlGaN for different values of content X

At the beam energies between 0 and 40 keV, the electrons penetrate into GaN on a depth of about 0-10 m, but in AlGaN the penetration depth is smaller, that depends on Al mole fractions X (Fig.3)

The Cathodoluminescence signal decreases when the aluminum percentage increases, this decreasing may be explicated by the increasing in band gap energy (the possibility of recombination decreasing) (Fig.4).

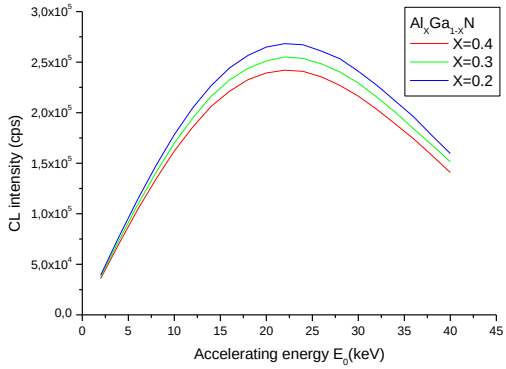

Fig.4. Cathodoluminescence signal as a function of accelerating energy for different values of content X

Figures 5 and 6 show the variation of minority carrier excess as a function of depth. The general form is Gaussian. The quantity of carrier excess depends on aluminium fraction.

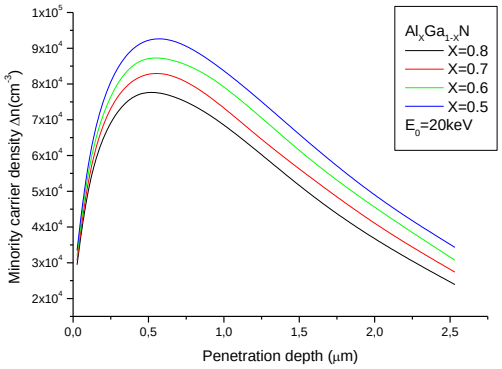

Fig.5. Minority carrier excess as a function of depth in AlGaN for different values of content X

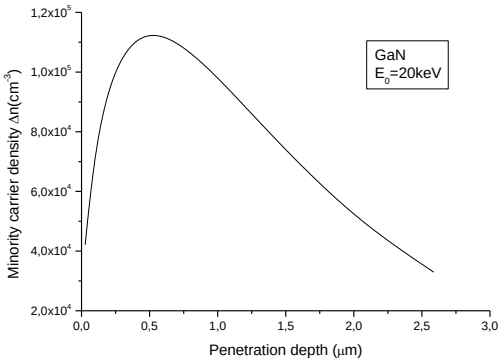

Fig.6. Minority carrier excess as a function of depth in GaN

4. Conclusions

The dependence of the cathodoluminescence signals on aluminum mole fraction is calculated and shows the cathodoluminescence signals decreases when the aluminum mole fraction increases.

A process of varying the elemental components of the semiconductor alloy in a controlled way to achieve a desired band gap that can emit a desired wavelength of radiation.

Finlay, the Al mole fraction is a critical parameter which determines the emission wavelength in AlGaN light-emitting diodes.

The band gap energy can be tailored to get desired visible light radiation.

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