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Cathodoluminescence study of undoped GaN films: Experiment and calculation

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ABSTRACT

In this paper, we report the theoretical and experimental results of cathodoluminescence (CL) from GaN layers grown at 800 °C by metal organic vapor phase epitaxy (MOVPE) on silicon substrate. The CL spectra recorded at room temperature reveal the near band-edge emission at 3.35–3.42 eV and a broad yellow luminescence at 2.2 eV. The CL depth analysis at constant power excitation shows inhomogeneous CL distribution in depth of these emissions as the electron beam increases from 3 to 25 keV. There appears a blue shift of the CL band-edge peaks with increasing sample depth. This behavior is explained by a change of the fundamental band gap due to residual strain and the local temperature rise under high electron beam excitation. The simulation of the CL excitation and intensity is developed using a consistent two-dimensional (2-D) model based on the electron beam energy dissipation and taking into account the effects of carrier diffusion, internal absorption and the recombination processes in GaN. The influence of electron beam local heating and respective strain effects on the CL signal are also discussed. A comparative study between experimental and simulated CL spectra at room temperature was performed.

1. Introduction

Cathodoluminescence (CL) spectroscopy has been recognized as an adequate tool to investigate the structural and optical properties of semiconductors and optoelectronic devices [1,2]. The scanning mode of CL is widely used to study the strains and morphology of epitaxial III–V semiconductor films [3–5]. Hildebrandt et al. [6] have investigated the recombination activity of dislocations in grown GaAs and GaP films by means of combined CL and electron beam-induced current (EBIC). From temperature-dependent CL analysis, they determined the activation energy of 11 meV for the defect emission in n-GaAs samples. Barjon [7] and Zarem [8] have used the CL measurements to determine the carrier diffusion length in GaAs/AlGaAs and GaN/AlGaN quantum wells.

Previously, many CL theories have been dedicated to simulate the CL emission phenomena [9–11]. Jones et al. [9] have developed a one-dimensional (1-D) model for the dependence of CL intensity in n-type GaAs with temperature in the range 150–500 K.

Djemel et al. [11] have applied the CL technique to study the effect of surface defects on the CL intensity from GaAs samples. The CL intensity is obtained by integration over the product of the excess minority carriers in time and the electron absorption

$$I_{CL} \approx \int_{z_d}^{\infty} \frac{\Delta n(z)}{\tau_n} \exp(-\alpha_b z)\, dz \quad (1)$$

where Δn are the excess minority carriers in the neutral region, τ_n the electron lifetime constant, z_d the depletion width and α_b the luminescent absorption coefficient.

Knobloch et al. [12] have suggested a simple but handsome model to investigate the influence of internal absorption on the CL emission as a function of electron beam energy. They modulated

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the collected CL by the convoluted integral

$$L_{\text{ext}}(h\nu) = \frac{1}{\sigma\sqrt{2\pi}} \int_0^{1.1R_\kappa} g(z) I(z, h\nu) \exp\left(-\frac{(h\nu - E_{\text{exc}})^2}{2\sigma^2}\right) \mathrm{d}z \qquad (2)$$

where $g(z)$ is the electron–hole pair generation function, $I(z,h\nu)$ the transmission through the layer of thickness z, E_{exc} the energy of excitonic emission, R_κ the primary electron range and σ the parameter of the Gaussian broadening. They observed a red shift of the band-edge (BE) luminescence of GaN of about 30 meV when the beam energy increases from 5 to 25 keV. The authors explained this behavior by the internal absorption tail at the BE [12].

In this regard, we have developed a theoretical model for calculating the CL intensity taking into account the effects of carrier diffusion, internal absorption, the recombination processes and the influence of the temperature increase due to electron beam heating. CL measurements are compared with the simulated spectra recorded at room temperature (RT) and liquid nitrogen temperatures (LNT) for undoped n-type GaN samples.

2. Experimental

The GaN samples used in this experiment were grown by metal organic vapor phase epitaxy (MOVPE) on the Si ⟨1 0 0⟩ substrates. Details of growth are found elsewhere [13,14]. The thicknesses of GaN layers #S1 and #S2 are 1.6 and 2.4 μm, respectively. Analysis of X-ray diffraction spectra shows that the layers are polycrystalline with preferential growth of the ⟨0 0 0 2⟩ hexagonal structure. The SEM investigations revealed a rough surface covered by randomly and well-developed GaN crystallites [14]. These samples are non-intentionally doped, having electron concentrations in the range 10^{17}–10^{18} cm^{-3}. The diffusion lengths of the minority carriers (holes) are determined by EBIC where its value was about 0.72 μm [15].

The CL measurements were performed in a digital scanning electron microscope (SEM) (Zeiss DSM 960). The CL spectra over the wavelength 200–800 nm, i.e. (1.5–6.2 eV), are detected via a parabolic mirror collector and analyzed with a Spex-270 M spectrograph and then registered by a Princenton Instr., EEV 1024×256 charge-coupled device (CCD) camera in single-shot technique of 1 s and with a spectral resolution of 4 nm. The overall spectral efficiency of the CL spectra registration shows a nearly constant plateau over the whole UV-red region (300–750) nm decaying only at the margins (200 and 800) nm to nearly 25% and 50%, respectively. Thus, a correction of directly measured spectra was not necessary and was not carried out. A cooling and heating temperature stage changes the sample temperatures between 80 and 670 K. In general, the CL excitation was performed with electron energies of 2–30 keV and beam currents of 200 nA in the TV scanning mode over an area of $(106 \times 110)\,\mu\text{m}^2$. This corresponds to an electron beam current density $j_o = 2\,\text{mA/cm}^2$. With 512×512 pixels, the scanning beam focus of a radius $d_o = 2\,\mu\text{m}$ is strongly (90%) overlapping from pixel to pixel and guarantees a homogeneous excitation over the excited area. The information from the lateral resolution of CL mapping in an SEM can be extended by a spatial depth analysis of varying the primary electron energy E_o and thus the excitation range. For practical use, the most convenient method, e.g. for CL depth analysis, is the constant power method, where the product of beam energy E_o and current I_o is kept constant ($E_o I_o$ = constant). In this case, the CL intensity measured versus E_o would remain constant when assuming a homogeneous depth distribution of luminescence centers. Deviation of such a behavior is easy to detect and to interpret.

3. Model theory

Here, we present the general theory of the CL induced by electron beam bombardment. The incident electron beam is focused perpendicular to the specimen surface, see Fig. 1. The generated electron–hole pairs can diffuse through the material, and then recombine to emit photons in the UV–visible–IR range.

The steady-state continuity equation in the case of low injection is described by

$$\nabla^2[\Delta p(x,z)] - \frac{\Delta p(x,z)}{L_p^2} = -\frac{1}{D_p} g(x,z) \qquad (3)$$

where Δp is the minority carrier (holes) concentration, L_p the hole diffusion length, $g(x,z)$ the spatial generation rate and D_p the hole diffusion coefficient.

The generation profile based on the electron energy dissipation and the lateral diffusion of charge carriers has the form [16]

$$g(x - x_o, z) = \frac{E_o(1-\eta)}{E_p(T)\sqrt{\pi}} \frac{1}{R_\kappa L_p} \frac{I_o}{q} \left\{ 0.6 + 6.21\left(\frac{z}{R_\kappa}\right) - 12.4\left(\frac{z}{R_\kappa}\right)^2 + 5.69\left(\frac{z}{R_\kappa}\right)^3 \right\} \exp - \left(\frac{x - x_o}{L_p}\right)^2 \qquad (4)$$

where $E_p(T) \approx 3E_g$ is the energy needed to create one electron–hole pair, E_g the band-gap energy, E_o the incident beam energy, and η the backscattered electron coefficient. R_κ is the maximum electron range depending on the incident beam energy E_o and the mass density ρ of the target [17]

$$R_\kappa = (0.052/\rho) E_o^{1.75}.$$

The boundary conditions associated with the physical model (Fig. 1) are

$$D_p \left(\frac{\partial \Delta p}{\partial r}\right)_{r=0} = V_s \Delta p \qquad (5)$$

where r means x or z abscises and V_s the surface recombination velocity.

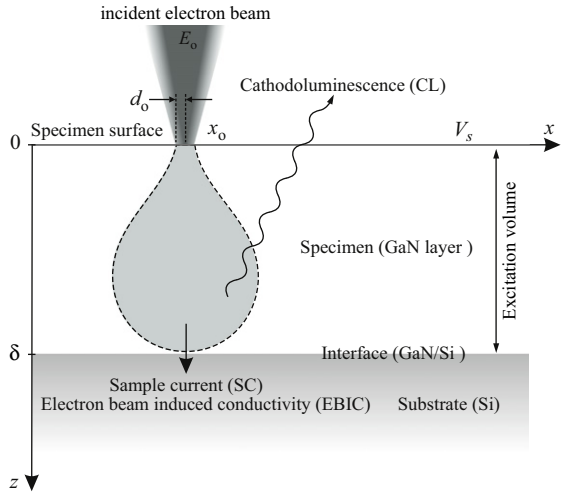

Fig. 1. Schematic presentation of spatial CL excitation by electron beam irradiation.