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Cathodoluminescence investigations of GaAs thin layers

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Abstract

In this work, we report the theoretical results of cathodoluminescence (CL) for GaAs layer. The simulation of the CL excitation and intensity is developed using 2-D model based on the electron beam energy dissipation and taking into account the effects of carrier diffusion, internal absorption and the recombination process in the semiconductors.

We have investigated the influence of the electron beam conditions (energy, current and beam diameter) and some physical parameters (absorption coefficient, gap energy) on the CL intensity. Results allow us particularly to predict the intensity evolution and shift of CL peak emitted near the fundamental energy gap as a function of the electron beam current and energy. A comparative study between simulated and experimental CL spectra at low temperature is realized.

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1. Introduction

The cathodoluminescence (CL) technique has frequently been used in the scanning electron microscopy (SEM) to study semiconductor materials. It's particularly used to provide valuable information on the luminescence properties such as composition, optical quality and doping levels of GaAs, GaN and related films [1]. Henceforth, many theories have been proposed to simulate the CL phenomena [2-4].

Barjon et al. [5] and Zarem et al. [6] have used the CL measurements to determine the carrier diffusion length in GaAs/AlGaAs and GaN/AlGaN quantum wells. Jones et al. [7] have developed a one-dimensional model for the dependence of CL intensity in n-type GaAs with temperature in the range 150-500 K. Djemel et al. [8] have applied the CL technique to study the effect of surface defects on the CL intensity from GaAs samples. Knobloch et al. [9] have suggested a simple model to examine the influence of internal absorption on the CL emission as a function of electron beam energy. The authors explained the red shift observed by the internal absorption tail at the band-edge.

In this paper, we report a 2 D model based on the electron energy dissipation and taking into account the effects of carrier diffusion, internal absorption, the recombination processes and the influence of the temperature increase

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due to electron beam heating. We investigated the influence of the electron beam conditions (energy, current and diameter beam) and some physical parameters (absorption coefficient, gap energy) on the CL intensity for the GaAs sample.

2. Model theory

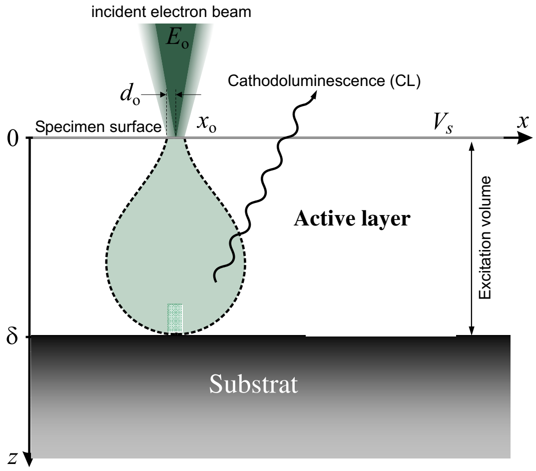

Fig. 1. Schematic presentation of spatial CL excitation by electron beam irradiation.

In this section, we present the general theory of the CL induced by the electron beam bombardment. The steady state continuity equation in the case of low injection is described by:

$$\nabla^2\left[\Delta m(x,z)\right]-\frac{\Delta m(x,z)}{L_m^2}=-\frac{1}{D_m}g(x,z) \tag{1}$$

Where Δm is the minority carrier (electrons or holes) concentration, L_m is the (electron or hole) diffusion length, g(x,z) the spatial generation rate and D_m is the carrier diffusion coefficient.

The generation profile based on the electron energy dissipation and the lateral diffusion of charge carriers has the form [10-11]:

$$g(x-x_0,z)=\frac{E_0(1-\eta)}{E_p(T)\sqrt{\pi}}\frac{1}{L_m}\frac{I_o}{q}\times\frac{1}{R_\kappa^2}\left(0.6+6.21(\frac{z}{R_\kappa})\ -\ 12.4(\frac{z}{R_\kappa})^2+5.69(\frac{z}{R_\kappa})^3\right)\times\exp-\left(\frac{x-x_0}{L_m}\right)^2 \tag{2}$$

where Ep(T) ≈ 3Eg is the energy needed to create one electron-hole pair, Eg the band gap energy, E_o the incident beam energy, η is the backscattered electron coefficient, q is the elementary charge, R_κ is the maximum electron range and x_o is the surface beam position [12].

With appropriate boundary conditions associated [11] to the physical model, the general solution of the continuity equation (1) is:

$$\Delta m(x,z) = \frac{E_0(1-\eta)}{E_p(T)\sqrt{\pi}} \frac{1}{R_\kappa L_m} \frac{I_o}{q} \times \frac{1}{D_m} \sum_k \frac{l_k}{l_k w - \sin l_k w} \times \frac{\cos l_k (x - 0.5w)}{\mu_k \left(e^{\mu_k (H-\delta)} + k_H e^{-\mu_k (H-\delta)}\right)}$$

$$\times \left[\int_0^{R_\kappa} f\left(\frac{z'}{R_\kappa}\right) \times \left(e^{\mu_k(-z+z'-\delta+H)} - e^{\mu_k(-z-z'+\delta+H)} + k_H e^{\mu_k(z+z'-\delta-H)} - k_H e^{\mu_k(z-z'+\delta-H)}\right) dz' \right] \tag{3}$$

$$\times \int_0^w \exp - \left(\frac{x' - x_0}{L_m}\right)^2 \times \cos l_k (x' - 0.5w)\, dx'$$

Where $\mu_k = \sqrt{\frac{1}{L_m^2} + l_k^2}$ and $k_H = \frac{\mu_k - \frac{V_H}{D_m}}{\mu_k + \frac{V_H}{D_m}}$

l_k is the solution of transcendent equation: $\mathrm{tg}\frac{w\, l_k}{2} = \frac{V_s}{D_m} \frac{1}{l_k}$

Where δ is the thickness of the active layer sample, w is the lateral length, Vs is the recombinaison velocity and H is the sample thickness.

In this approach, we have considered the thermal effect induced by the electron beam bombardment as well. In fact, it is known that under high energetic electron beam conditions [13-14], the material can be heated leading to change of the fundamental gap and thus to shifts of the band-edge CL transitions toward the low or high photon energies. Consequently, the expression of the temperature variation will have the form [13, 15]:

$$\Delta T = \frac{0.82}{\sqrt{\pi}} \frac{I_O V_O}{C_T d_O} \tag{4}$$

where I_o is the electron beam current (A), V_o is the beam voltage (V), d_o is the beam diameter (cm) and C_T is the thermal conductivity ($W.cm^{-1}. K^{-1}$). For an electron beam with I_o= 200 nA, V_o = 20 000V and d_o= 2 µm, the temperature increase in GaAs can reached 18.5 K.

For the energy gap, an empirical expression is used [16]:

$$E_g(T) = E_{go}(0K) - \frac{5.405\times10^{-4}\times(T')^2}{(T') + 204} \tag{5}$$

Where Ego =1.519 eV is the energy gap at 0K for the pure GaAs sample, and T´ = T + ΔT.

The absorption coefficient has been described by Urbach [17]:

$$\alpha(T) = \alpha_0 \exp\left(\frac{h\nu - E_g(T)}{k_B T}\right) \qquad \text{for } h\nu < E_g \tag{6}$$

T is the absolute temperature and k_B is the Boltzmann's constant. For photon energies above the energy gap Eg, the absorption coefficient is assumed to be constant with a value $\alpha_o = 10^5$ cm^{-1}.

Theoretically, the extrinsic or intrinsic luminescence is described by the following expression [18]:

$$L_{um}(h\nu) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{\beta\,(h\nu - E_g(T+\Delta T) + E_i)^2}{2\sigma^2}\right) \tag{7}$$

E_i is the activation energy, σ the parameter of the Gaussian broadening and β is a corrected parameter corresponding to the full width at half maximum (FWHM) of each CL peak.

So, the CL intensity is given by the integration of the radiative recombination rate in equation (3) extended over the neutral region:

$$I_{CL}(h\nu) = \int_0^w \int_{R_\kappa}^H \frac{\Delta m(x,z)}{\tau_m} \times L_{um}(h\nu) \times \exp(-\alpha z)\, dx\, dz \tag{8}$$

3. Results

3.1: Effect of the electron beam energy.

The samples used in this study were 2.4 µm thick layers grown by metal organic chemical vapour deposition (MOCVD) at temperature T= 800 °C.

Fig.2 reports the variation of simulated spectra as a function of photon energy for different electron beam energy. When the beam energy rises from 5 to 10 keV, it shows an increase of the CL intensities. Above E_o=10 keV, the CL intensity decreases. Also it exists a displacement of the band edge peaks towards the low photon energy, in accordance with the results observed by Knobloch et al. [9] for the band-edge (BE) luminescence of GaN when the beam energy increases from 5 to 25 keV. This behavior is accentuated when the current intensity increases from 20 to 500 nA (see Fig. 3).

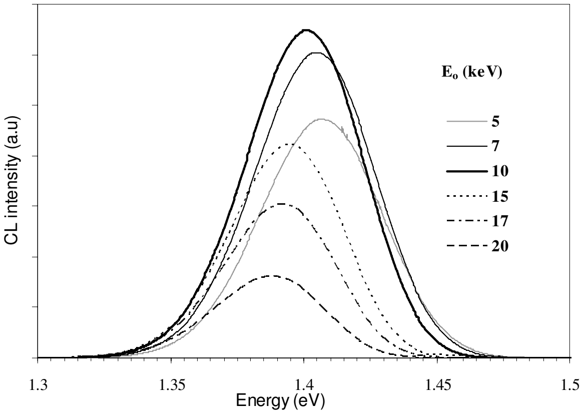

Fig. 2. Simulated CL spectra of the material GaAs (2.4 µm) obtained for different electron beam energies (T= 297K, d_o= 2 µm, I_o = 200 nA).

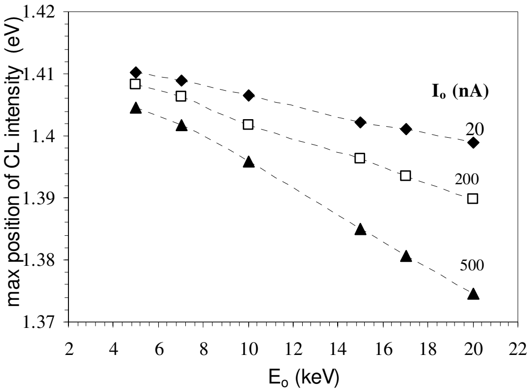

Fig. 3. Maximum position of CL intensity as function of electron beam energy at different current intensities.

3.2: Effect of the current intensity

Fig. 4 reports the variation of simulated CL spectra for different current intensity. It shows an increase of the CL intensities when the current intensity is varied from 20 to 200 nA. It is seen also a feeble displacement of the band edge peaks towards the low photon energy [3, 13]. We attribute the decrease of energy position to the shrinkage of band energy caused by the electron beam heating.

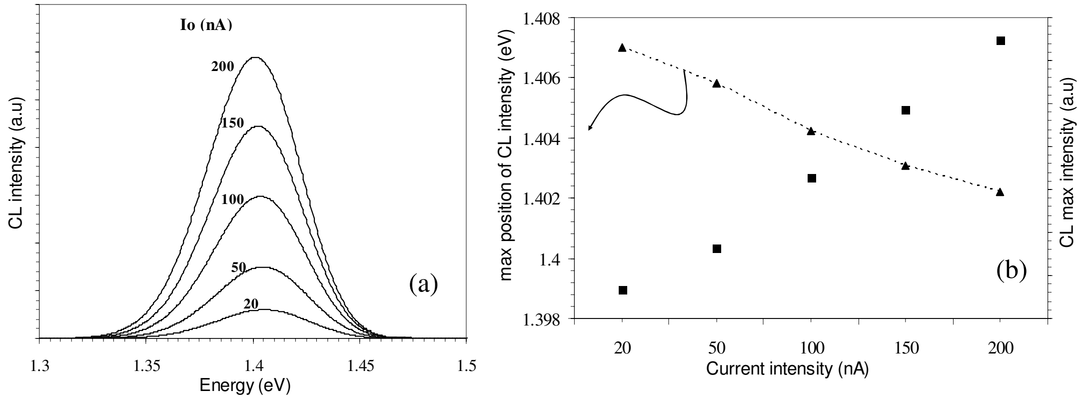

Fig. 4. Simulated CL spectra of GaAs (a) and CL position for band edge peak (b) obtained for different current intensity (T = 297 K, E_o = 10 keV).

3.3: Effect of the absorption coefficient

Fig. 5 presents the variation of simulated spectra as a function of energy photon for different absorption coefficient. We note a decrease of the CL intensities of the band edge peaks when the absorption coefficient increases. This behaviour was caused mainly by the attenuation of the transmitted light in the bulk material.

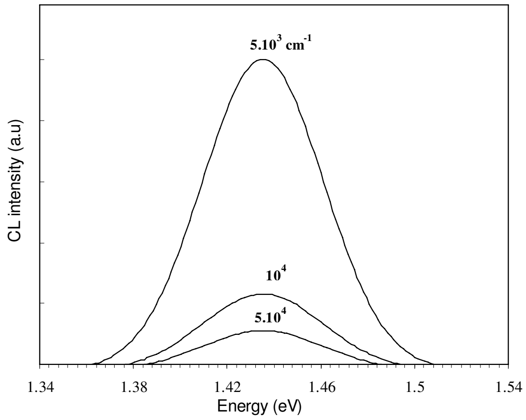

Fig. 5. Simulated CL spectra of the material GaAs obtained for different absorption coefficient (T = 297 K, E_o = 20 keV, I_o = 200 nA).

3-4 Effect of the beam diameter.

Fig. 6 shows the variation of CL spectra of the 2.4 µm thick sample for different values of beam diameter. The spectra show CL peak at 1.358-1.4 eV. When the beam diameter increases from 0.1 to 1 µm, the band edge peaks shift to higher photon energies by 9-15 meV. Recently, we have observed similar phenomena in CL emissions from GaN material [19]. We attribute the observed blue-shifts to the increase of the energy gap induced mainly by the local temperature variation of the semiconductor target.

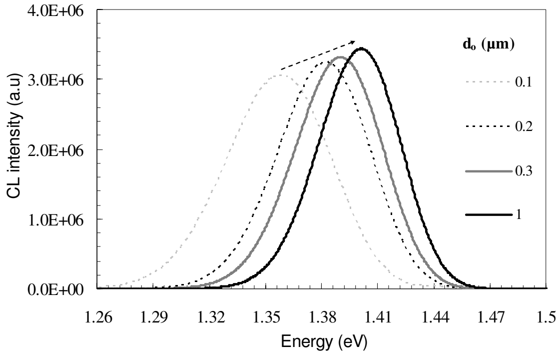

Fig. 6. Simulated CL spectra of the material GaAs obtained for different beam diameter. (T = 297 K, I_o = 100 nA, E_o = 10 keV).

4. Comparison

The comparative study between experimental and simulated CL spectra at low temperature is presented in figure 7. The experimental CL spectrum exhibits a peak at 1.508 eV with a full width at half-maximum (FWHM) of 13 meV assigned to band edge luminescence of GaAs. The theoretical and the experimental curves show good agreement in shape and position of the observed band edge peak. This proves that the proposed model is well validated by experimental data in the case of GaAs sample.

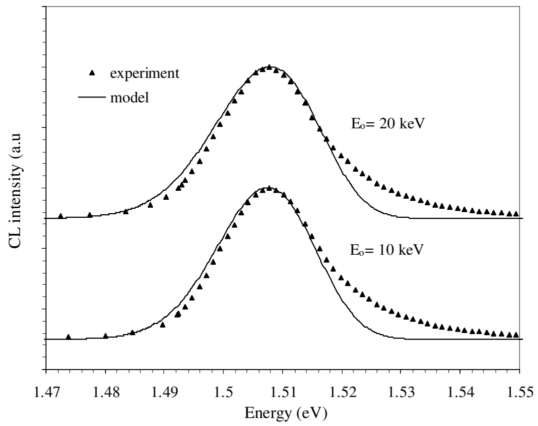

Fig. 7. Comparison of Low nitrogen temperature (77 K) CL spectra with the simulated ones from GaAs obtained for E_o = 10 keV and 20 keV (I_o = 200 nA, L_m = 0.7 µm, $V_s = 10^6$ cm.s^{-1}).

5. Conclusion

In the present work, we report the influence of electron beam local heating on the CL signals in GaAs samples. Results of simulation show red-shifts of the CL band edge peaks with increasing the electron beam current and energy. The variation beam diameter leads to displacement of the BE emission towards high photon energy. These behaviors are explained by a change of the fundamental band gap due to the local temperature variation under the high electron beam excitation. As the absorption coefficient is increased, we assisted to important decrease of the CL intensities which is caused by light losses in the material depth. A comparative study between experimental and simulated CL spectra in the case of GaAs sample, permitted a validation of our model.

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