Study of surface defects in GaAs by cathodoluminescence: calculation and experiment

2000 J. Phys.: Condens. Matter 12 10343

(http://iopscience.iop.org/0953-8984/12/49/338)

J. Phys.: Condens. Matter **12** (2000) 10343–10347. Printed in the UK PII: S0953-8984(00)17585-X

Study of surface defects in GaAs by cathodoluminescence: calculation and experiment

A Djemel†, A Nouiri† and R-J Tarento‡

† Department of Physics, University of Constantine, 25000 Algeria
‡ Université Paris-sud, Bâtiment 510, 91405 Orsay, France

Received 29 September 2000

Abstract. In this work, we propose a model for self-consistent calculation of the cathodoluminescence intensity, which has been used to study surface defects in GaAs materials. In this model, we have taken into account the influence of surface defects on the electron beam parameters (energy E_o, intensity I_p) and the depletion region (Z_d). Without introducting the concept of a 'dead layer', we have calculated the dependence of the CL intensity on the surface parameters (defect density N_t and energy level associated E_t). By comparison of the experimental results with the theoretical curves, some surface parameters have been derived.

1. Introduction

In all studies of cathodoluminescence (CL), the authors can differentiate between surface and bulk phenomena. The recombination of excess carriers at the free semiconductor surface under cathodic excitation is characterized by the recombination velocity v_s [1]. Some correlations between the CL intensity and the surface properties are explained by introduction of the concept of a 'dead layer' [2–5]. The problem of interest is the dependence of the CL intensity on the physical parameters characterizing the surface defects, i.e. density N_t, energy E_t.

The dependence of v_s on N_t, E_t, and capture cross section σ in the case of grain boundaries (GBs) has been studied [6], but the analytical expression given is not valid for the free surface. The complex surface attributes of GaAs have been studied in detail [7]. The authors have investigated low temperature excitonic behaviour and compared the CL response with photoluminescence (PL).

A theoretical study of the electronic surface properties of GaAs is detailed in [8]; the depletion region is assumed to be the result of the charge associated with the defect surface, which depends on the injection conditions (i.e. primary intensity I_p, electron beam energy E_o). Then, the dependence of the CL intensity on some physical parameters is studied [9, 10]. In this paper, we have used our model [8] to study surface defects which are characterized by defect density N_t and an associated energy level E_t. The recombination at the surface is explained by E_t, which is determined by comparison of the experiment results with theoretical curves for different surface treatments.

2. Theory

The theory assumes that the semiconductor GaAs is p type with acceptor concentration N_a. The free surface of the semiconductor is defined as a density of defects all with one energy

0953-8984/00/4910343+05$30.00

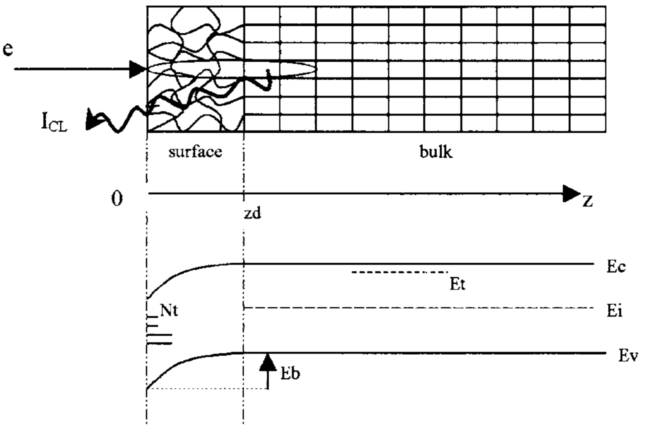

Figure 1. Schematic representation of the energy band diagram and the surface defects used in the proposed model.

level, located at E_t above the intrinsic Fermi energy (E_i) (figure 1). The surface recombination is treated in the Shockley–Read–Hall mechanism for non-equilibrium conditions.

The absolute charge of the surface Q is given by:

$$Q = N_a Z_d e = N_t(1-f)e \qquad \text{and} \qquad Z_d = \frac{N_t}{N_a}(1-f). \tag{1}$$

The depletion region width Z_d increases linearly with N_t and depends on E_t by means of f. The occupation probability of the donor energy level f is given by [11]:

$$f = \frac{\Delta n(0) + n_0 + n_i \exp((E_i - E_t)/kT)}{\Delta n(0) + n_0 + \Delta p(0) + p_0 + 2n_i \cosh((E_t - E_i)/kT)} \tag{2}$$

where $\Delta n(0)$ and $\Delta p(0)$ are the electron and hole excess carrier concentrations at the surface, respectively, and n_i is the intrinsic carrier concentration.

The electron (hole) concentration at the surface n_0 (p_0) is given by:

$$n_0 = \frac{n_i^2}{N_a}\exp\left(\frac{E_b}{kT}\right) \qquad p_0 = N_a \exp\left(-\frac{E_b}{kT}\right) \tag{3}$$

where E_b is the barrier height, which is given by:

$$E_b = \frac{eN_a Z_d^2}{2\varepsilon}. \tag{4}$$

The barrier height depends on N_t and E_t by means of Z_d.

The continuity equations of both majority and minority carriers are solved in the neutral (bulk) and the depletion (surface) regions (figure 1).

The continuity equation can be written in the following form:

$$\operatorname{div} \vec{J} = G(r) - R(r) \tag{5}$$

where $G(r)$ is the generation rate and $R(r)$ is the recombination rate.

In the present calculation, we consider a one-dimensional problem, and the recombination is neglected in the depletion region. Thus, the continuity equation for electron excess $\Delta n(z)$ and hole excess $\Delta p(z)$ in the depletion region is recast in the following form:

$$\left\{ \begin{array}{l} -\dfrac{\mathrm{d}^2\Delta n(z)}{\mathrm{d}z^2} + 2\alpha(z - z_d)\dfrac{\mathrm{d}\Delta n(z)}{\mathrm{d}z} + 2\alpha\Delta n(z) = \dfrac{G(z)}{D_n} \\ -\dfrac{\mathrm{d}^2\Delta p(z)}{\mathrm{d}z^2} - 2\alpha(z - z_d)\dfrac{\mathrm{d}\Delta p(z)}{\mathrm{d}z} - 2\alpha\Delta p(z) = \dfrac{G(z)}{D_p}. \end{array} \right. \tag{6}$$

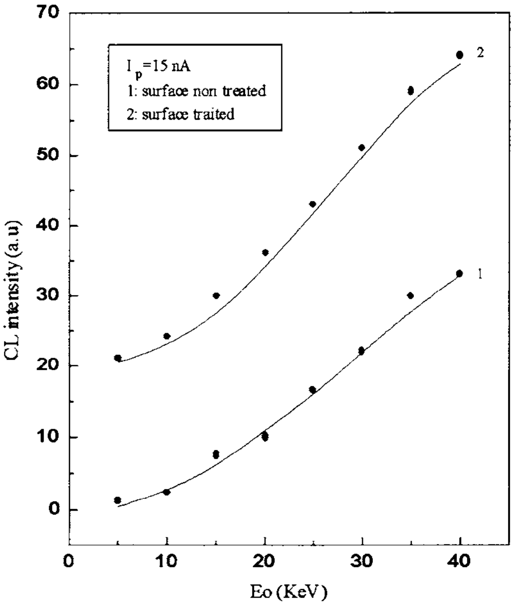

Figure 2. CL intensity measurements as a function of acceleration energy E_o before and after surface treatment for non-deformed p-GaAs. Full lines are the results of the proposed model: (1) $E_t = 1.30$ eV, (2) $E_t = 1.33$ eV. ($N_t = 2 \times 10^9$ cm^{-2}, $\sigma = 10^{-16}$ cm^2, $L_n = 0.70$ μm, $\alpha_b = 8 \times 10^3$ cm^{-1}.)

Using the Einstein relation ($D/\mu = kT/e$), α becomes equal to $N_a e^2/2\varepsilon kT$. Here $D_{n(p)}$ is the electron (hole) diffusion coefficient, and $\mu_{n(p)}$ is the mobility of an electron (hole). The analysis, assumptions and the solution of the continuity equations (6) are detailed in [8].

In the neutral region, the carriers flux is due to the diffusion component of the minority carriers, and the majority carriers follow this in order to maintain the local charge neutrality. The continuity equation is:

$$-D_n \frac{\mathrm{d}^2 \Delta n(z)}{\mathrm{d}z^2} = G(z) - \frac{\Delta n(z)}{\tau_n} \tag{7}$$

where τ_n is the lifetime of minority carriers which is related to diffusion length (L_n) by

$$L_n = \sqrt{D_n \tau_n}. \tag{8}$$

The general solution of the continuity equation (7) is

$$\Delta n(z) = B_n \exp\left[-\frac{(z - z_d)}{L_n}\right] + \frac{L_n}{2D_n} \int_{Z_d}^{z} G(z') \left\{ \exp\left(-\frac{|z - z_d|}{L_n}\right) - \exp\left[-\frac{(z + z' - 2z_d)}{L_n}\right] \right\} \mathrm{d}z' \tag{9}$$

where B_n is the electron concentration at the limit of the depletion region

$$B_n = \Delta n(z = z_d). \tag{10}$$

The cathodoluminescence intensity I_{cl} comes only from the recombination of excess carriers in the neutral region (the recombination is neglected in the depletion region) and it is given by

$$I_{cl} \propto \int_{z_d}^{\infty} \frac{\Delta n(z)}{\tau_n} \exp(-\alpha_b z) \, \mathrm{d}z. \tag{11}$$

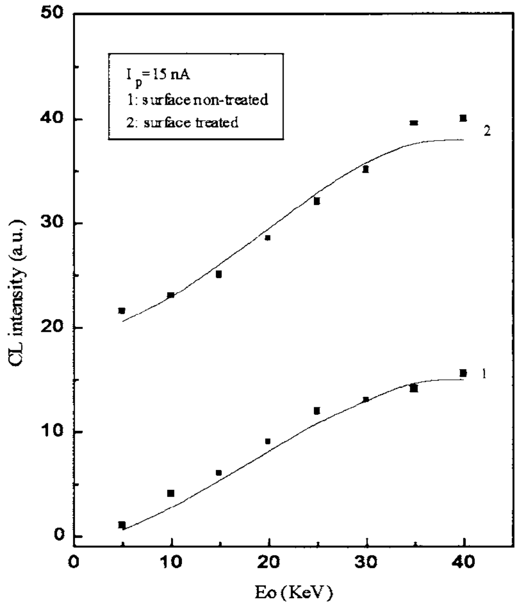

Figure 3. CL intensity measurements as a function of acceleration energy E_o before and after surface treatment for deformed p-GaAs. Full lines are the results of proposed model: (1) $E_t = 1.30$ eV, (2) $E_t = 1.33$ eV. ($N_t = 2 \times 10^9$ cm^{-2}, $\sigma = 2 \times 10^{-16}$ cm^2, $L_n = 0.55$ μm, $\alpha_b = 10^4$ cm^{-1}.)

Here, α_b is the absorption coefficient. The CL intensity depends on surface defects by means of Z_d.

3. Results and discussion

Two samples of p-GaAs have been investigated, deformed and non-deformed, with acceptor concentration $N_a = 10^{16}$ cm^{-3}. Two surfaces are compared: one is non-treated and the other is chemically polished with H_2SO_4:H_2O_2:H_2O (9:1:1) for two minutes and finally rinsed with deionized water.

CL measurements have been performed at room temperature. The primary electron beam intensity was 15 nA, with an electron energy ranging from 5 to 40 keV.

The numerical results show that the surface defects (characterized by N_t and E_t) modify the profiles of excess carriers, which themselves affect the CL intensity [9, 10]. The experimental dependence on electron beam energy of CL intensity obtained for non-deformed p-GaAs is given in figure 2. The results for the deformed sample are shown in figure 3. The full lines are the result of model calculations. In all cases, after chemical treatment of the surface, the CL intensity increases. This behaviour is due to the change of the surface recombination velocity. In our case, this change is due to the energy level E_t, which explains the surface recombination. For this reason, the adjustment between the numerical results and experimental data has been obtained by a change in energy level E_t. The surface recombination becomes important when the energy level E_t is near to the middle of the gap.

For the deformed sample, we have found the same behaviour. The treated surface presents a low surface recombination, and the energy level E_t is close to the conduction band. But some changes have been introduced to the capture cross-section ($\sigma = 2 \times 10^{-16}$ cm^{-2}), the absorption coefficient ($\alpha_b = 10^4$ cm^{-1}) and the diffusion length ($L_n = 0.55$ μm). The capture cross section is generally linked to both defect and its environment [12]. The defects introduce a stress field which itself modifies the gap [13]. Similarly, extended defects which have been introduced by high temperature plastic deformation reduce the CL intensity [14, 15].

4. Conclusion

A model of self-consistent calculation of the free semiconductor surface under cathodic excitation is proposed. In this model, the recombination at the surface is characterized by an energy level E_t associated with surface defects (N_t) and a capture cross-section σ. The comparison between the numerical results and experimental data gives a good estimation of these parameters.

References

[1] Yacobi B G and Holt D B 1990 *Cathodoluminescence Microscopy of Inorganic Solids* vol 2 (New York: Plenum)
[2] Wittry D B and Kyser D F 1966 *J. Soc. Japan* **21** 312
[3] Wittry D B and Kyser D F 1967 *J. Appl. Phys.* **38** 375
[4] Rao-Sahib T S and Wittry D B 1969 *J. Appl. Phys.* **10** 3745
[5] Hergert W, Reck P, Pasemann L and Schreiber J 1987 *Phys. Status Solidi* a **101** 611
[6] Marfaing Y and Maurice J-L 1991 *Springer Proc. Phys.* **54** 205
[7] Myhajlenko S, Davito D B, Puechner R A and Edwards J L 1994 *Phil. Mag.* B **69** 553
[8] Djemel A, Tarento R-J, Castaing J, Marfaing Y and Nouiri A 1998 *Phys. Status Solidi* a **168** 425
[9] Nouiri A, Djemel A and Tarento R-J 1999 *Algerian J. Adv. Mater.* **3** 27
[10] Nouiri A, Djemel A and Tarento R-J 2000 *Microelectron. Eng.* **51/52** 151
[11] Tarento R-J and Marfaing Y 1992 *J. Appl. Phys.* **71** 4997
[12] Bourgoin J C and Coebett J W 1972 *Phys. Lett.* A **38** 135
[13] Djemel A, Castaing J, Heurtel A, Svob L and Marfaing Y 1987 *Phil. Mag. Lett.* **55** 239
[14] Djemel A, Castaing J, Visentin N and Bonnet M 1990 *Semicond. Sci. Technol.* **5** 1221
[15] Djemel A, Castaing J, Chevallier J and Henoc P 1992 *J. Physique* III **2** 2301