THEORETICAL STUDY OF CATHODOLUMINESCENCE OF CdTe INFLUENCE OF BULK PARAMETERS.

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Abstract

The effect of bulk parameters (¬diffusion length (Ln), absorption coefficient (α) and acceptor concentration (Na)) on the cathodoluminescence intensity (ICl) of p type CdTe has been theoretically investigated. To do this a self-consistent calculation method of (ICl) has been used. The obtained results show that ICl decreases when Ln and α increase up to a certain excitation energy E0, and then begins to decrease. The maximum of the ICl = f(E0) curves shifts towards high energies.

Keywords: *Cadmium Telluride, Cathodoluminescence, Bulk parameters, Self consistent method.*

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I. INTRODUCTION

The use of the scanning electron microscopy in cathodoluminescence mode (SEM-CL) has a great merit for the investigation of materials at a microscopic scale.

The cathodoluminescence (Cl) is a very powerful technique which allows a spatial and spectral characterization of semiconductors. It has been widely used for the determination of parameters such as the diffusion length of the minority carriers, the absorption coefficient and the surface recombination velocity [1-7].

However, a determination, as accurate as possible, of these parameters needs an exact description of the Cl signal generation.

Until now, little attention has been paid to the theoretical study of the cathodoluminescence on cadmium telluride, as well as, the Cl dependence with the material parameters is much less developed.

In addition, there is no detailed theoretical information and also no results available on the influence of the bulk parameters on Cl.

Most previous theoretical studies of the Cl relate to the case of GaAs [8, 9]. That is why this work is of particular importance.

The study is based on a theoretical model allowing the calculation of the Cl intensity [10,11], in order to investigate the influence of bulk parameters (diffusion length, absorption coefficient and doping concentration) of the material, on Cl signal.

The role of these parameters has been determined through the discussion of the curve profiles of the signal versus the beam acceleration energy.

2. THE THEORETICAL MODEL

The modeling of cathodoluminescence phenomena and the approximations used are based on the following assumptions:

- The studied sample is CdTe p type: it is considered semi-infinite, homogeneous, and divided on two regions, the depletion region (at the surface) and the neutral region (in the volume).

- It is assumed that there is no radiative recombination in the depletion region, and that the electron-hole pairs generated by the incident electron beam, normal to the surface, are separated on two opposite directions due to the existence of the electric field [8].
- The capture coefficient of electrons and holes is the same.
- The defects considered are surface defects. They have: an energy level E_t, a concentration N_t and a charge Q.
- A self-consistent method has been used for the calculation of the thickness Z_d.

- In the neutral region, we assume that the defects don't affect the minority carrier concentration.

- The minority carriers, generated by the electron beam (characterized by the current intensity I_p and the incident energy E_0) have steady-state diffusion.

- The analytical form of the energy dissipation function, is that proposed by Wu and Wittry [12], it is a modified Gaussian approximation, given by:

$$\phi(u) = A.\exp\left[-\left(\frac{u-u_0}{\Delta u}\right)^2\right] - B\exp\left(-\frac{bu}{u_0}\right) \qquad (1)$$

Δu, u_0, b, B/A are constants, given in the case of CdTe by the following values [11]:

$\Delta u = 0.17$, $u_0 = 0.057$, $b = 3$, $B/A = 0.5$

u is the normalized penetration ($u=\rho.z/R_e$), ρ the density of the material (in g/cm^3) and R_e the maximum penetration

depth of electron, given by K. Kanaya and S. Okayama [13]:

$$\mathrm{Re}(\mu m) = 0.0276 \frac{A}{\rho Z^{0.889}} E_0^{1.67} \qquad (2)$$

Where A is the atomic weight (A_{CdTe} = 240), Z the atomic number (Z_{CdTe} = 50), E_0 being the incident energy in keV, ρ the density of the material (ρ_{CdTe} = 6.1g/cm^3).

3. RESOLUTION OF THE CONTINUITY EQUATION

To calculate the signal Cl, we have to resolve the continuity equation (3) of a steady-state on one dimension, which is the depth z in the neutral region.

$$div.\vec{J}_n = G_n(z) - R_n(z) \qquad (3)$$

Where $G_n(z)$ and R_n (z) are the generation and recombination rates of minority carriers, respectively, $\vec{J}_n$ the flux of the minority carriers, due to the diffusion component (gradient of concentration) only. $\vec{J}_n$ is given by:

$$\vec{J}_n = -D_n \, grad(\Delta n) \qquad (4)$$

Where D_n is the coefficient of diffusion.
For the low injection case, for a p-type semiconductor (Δp and Δn << p_0), the recombination rate will be given by:

$$R_n = \frac{\Delta n(z)}{\tau_n} \qquad (5)$$

Where τ_n is the electron lifetime, related to the diffusion length L_n and the diffusion coefficient D_n by: $\tau_n = \frac{L_n^2}{D_n}$

The relationship between the generation rate and the function of the dissipation energy ϕ (u) is given by:

$$G(z) = \frac{\rho}{R_e}\phi(u) \qquad (6)$$

Taking into account the equations 4 and 5, the continuity equation can be rewritten as follows:

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

The solution of this differential equation is:

$$\Delta n(z) = B_n \exp\left[-\frac{(z - Z_d)}{L_n}\right] + \frac{L_n}{2.D_n}\int_{z_d}^{z} G(z')\left\{\exp\left(-\frac{|z - z'|}{L_n}\right) - \exp\left(-\frac{z + z' - 2Z_d}{L_n}\right)\right\}dz' \qquad (8)$$

Where B_n is a constant, giving the excess electron concentration at ($Z=Z_d$: $B_n = \Delta n|_{Z=Zd}$).

4. CALCULATION OF THE CL SIGNAL INTENSITY

The total luminescence emitted from the sample is the intensity of the cathodoluminescence signal (I_{Cl}) [7].

$$I_{Cl} = (1 - R)\int_V A'(z)\ \eta.\frac{\Delta n(z)}{\tau}.dz \qquad (9)$$

Where V is the sample volume, Δn (z) the concentration of the excess minority carriers, η the luminescence efficiency coefficient, equal to τ/τ_r, τ being the total lifetime given by: $1/\tau = 1/\tau_r + 1/\tau_{nr}$, τ_r and τ_{nr} being the radiative and nonradiative lifetime respectively, (1-R) is the transmission coefficient through the surface and R the reflection coefficient, which can be expressed from the refractive index *n* by:

$$R = \left(\frac{n-1}{n+1}\right)^2 \qquad (10)$$

For CdTe *n* is equal to 2.75.
A' (z) is the correction function of the optical losses at the depth z given by [14]:

$$A'(z) = \int_0^{\theta_c} \exp\left(\frac{-\alpha z}{\cos\theta}\right)\sin\theta \, d\theta \qquad (11)$$

where α is the absorption coefficient, θ_c the critical angle of total reflection on the surface, which depends on the refractive index of the material, we have:
$\sin\theta_c = 1/n$ [15].

If θ_c is not high enough, as is the case for CdTe (θ_c = 21°), we can approximate the relation (11) and obtain:

$$A'(z) \approx \exp(-\alpha.z) \qquad (12)$$

The calculation of I_{CI} was subject to the following approximations:

- The reflection coefficient will remain low as long as the critical angle of total reflection is low.
- The excitation by means of electron beam can be approximated by a point source situated in the volume.
- The correction function of energy losses is given by the formula 12.
- Only radiative processes in the neutral region are considered, the lifetime will be $\tau \approx \tau_r$.
- The generation of electron-hole pairs due to the absorption of the internal luminescence is assumed to be negligible.

Taking into account these approximations, the simplified model of weak excitation conditions, in the case of the band to band energy emission, was used. Thus the total Cl intensity is given by:

$$I_{Cl} \approx \int_{Z_d}^{+\infty} \frac{\Delta n(z)}{\tau_r}\exp(-\alpha.z)dz \qquad (13)$$

5. RESULTS AND DISCUSSION

The variation of the cathodoluminescence intensity (I_{Cl}) with the incident electron beam energy is shown in Fig.1. These curves are the best ones providing quantitative results.

The influence of L_n, α and Na parameters will be discussed in detail later in this work. The influence of the diffusion length can be seen on fig.1: for a given value of L_n, I_{Cl} increases until a maximum, reached for a certain value E_0, that moves significantly to high energies when L_n increases.

Generally I_{Cl} decreases with increasing L_n, due to the excess carriers, which take a long time for recombination.

The appearance of a maximum for all the three values of L_n is related, on one hand, to carriers recombination, which generate the Cl signal, and on the other hand, to the optical absorption of the material, which reduces the Cl intensity. We are in the presence of competition between two phenomena: the minority carriers recombination is dominant up to a maximum, reached for some value E_0, and then the optical absorption of the material becomes predominant. In addition, a shift of the maxima towards high energies is observed. It is explained, once again, in terms of recombination time: as soon as the L_n increases the time becomes longer and we need, therefore, more energy.

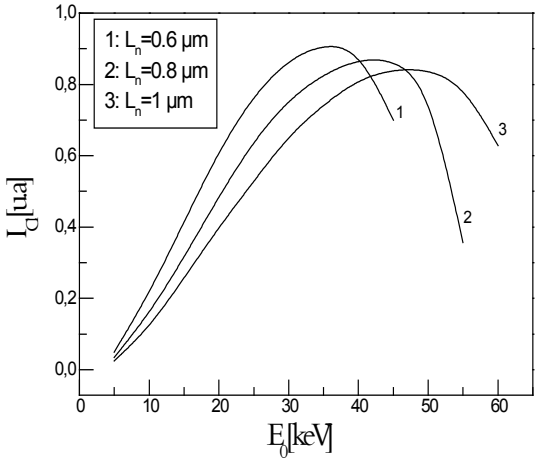

Figure 1. Variation of I_{Cl} intensity as a function of incident energy for different diffusion lengths. ($I_p=10^{-10}$A, E_t=1.3eV, $N_t=10^8$cm^{-2}, $N_a=10^{15}$cm^{-3}, $\alpha=10^4$cm^{-1}).

The absorption coefficient, as shown in Fig. 2, acts significantly on Cl. This latter decreases with increasing absorption coefficient. Generalizing, we can say that I_{Cl} would vanish for high values of α. Every curve has a maximum for a certain E_0, which shifts, weakly, towards high energies. This shift is explained in terms of diminution of α effect at high energies: the absorption is delayed in comparison with lower energies.

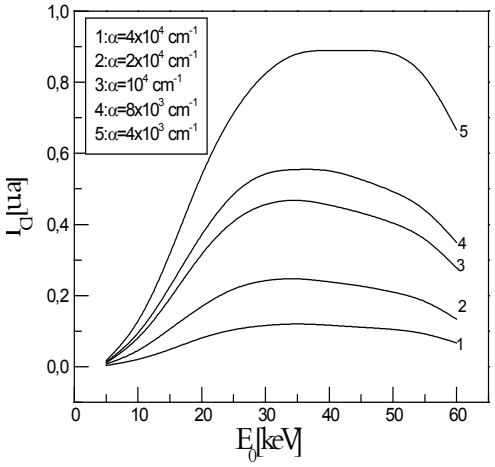

Figure 2. Variation of I_{Cl} intensity as a function of incident energy for different absorption coefficients. ($I_p=10^{-10}$A, E_t=1.3eV, L_n=1µm, $N_t=10^8$cm^{-2}, $N_a=10^{15}$cm^{-3}).

Figure 3 shows the influence of the doping concentration on I_{Cl}. We note that I_{Cl} decreases with increasing N_a up to a well determined value of incident beam energy. This can be explained by the rate of nonradiative recombination, which increases when N_a increases if we are in the low injection case. For high energies, the phenomenon is reversed because we are in high injection case. This explains why the curves and their maxima, of course, are shifted towards high energies.

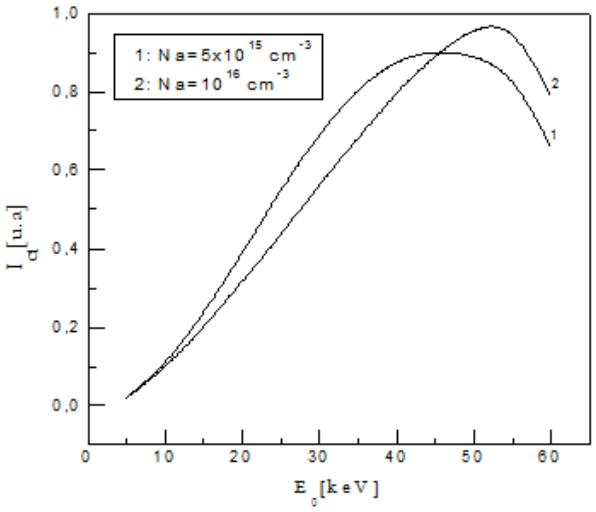

Figure 3. Variation of I_{Cl} intensity as a function of incident energy for different doping concentrations. ($I_p=10^{-10}$A, L_n=1µm, E_t=1.3eV, $N_t=10^8$cm^{-2}, $\alpha=10^4$cm^{-1}).

6. CONCLUSION

In this study the influence of the most important bulk parameters (diffusion length (L_n), absorption coefficient (α) and acceptors concentration (N_a)) on the cathodoluminescence intensity (I_{Cl}) of p type CdTe has been theoretically demonstrated.

All curves show the same behavior, and each has a maximum, due to two competing phenomena, the first is the generation-recombination of electron-hole pairs, which increases the luminescence and dominates at low energies, the second is the absorption, which contributes to the decrease in luminescence, in particular, for high energy.

The obtained results indicate that the Cl makes a difference between the volume and surface phenomena: the influence of L, α and N_a parameters is more significant (great difference between the curves) for high energies, while for low energies this influence is weak.

By adjusting the theoretical and experimental curves quantitative values of the various parameters can be estimated.

The accuracy of the results led us to propose the model used in this study to predict experimental results by choosing the best conditions.

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REFERENCES

[1] N. L. Dmitruk, V. G. Litovchenko and G. H. Talat, The effect of the surface space charge region on the cathodoluminescence of semiconductors, *Surface Science* 72, (1978), 321-341.

[2] W. Hergert, P. Reck, L. Pasemann, and J. Schreiber, Cathodoluminescence measurements using the scanning electron microscope for the determination of semiconductors parameters, *Phys. Stat. Sol. a* 101, (1987), 611-618.

[3] C. H. Jacob Phang, K. L. Pey and S. H. Daniel Chan, A simulation Model for cathodoluminescence in the Scanning Electron Microscope, *IEEE Transactions on Electron Devices* 39, (1992),782-791.

[4] D. B. Wittry, D. E. Kyser, Measurement of diffusion lengths in direct-gap semiconductors by electron beam excitation, *J. Appl. Phys*. 38, (1967), 375-382.

[5] V.M. Leonov, A .G.Molchanov, Y.M. Popov and G.H. Talat, Investigation of the influence of surface annihilation of excitons on cathodoluminescence of CdS, *Sov. Phys. Semicond.* 10, (1976), 852-855.

[6] T. I. Kovtunuva, N.N. Mikheev, A. N. Polyakov, and M. A. Stepovich, On the possibility of the mathematical modeling of the dependence of cathodoluminescence intensity on the energy of beam electrons with the use of the power series approximation in the problem of identifying the parameters of semiconductor meterials, *J. Surf. Inv. X-ray, Sync. Neut. Tech.* 4, (2010), 778-783.

[7] F. Cléton, B. Sieber, R. A. Masut, L. Isnard, J. M. Bonard and J. D. Ganière, Photon recycling as the dominant process of luminescence generation in an electron beam excited n-InP epilayer grown on an n^+-InP substrate, *Semicond. Sci. Technol.* 11, (1996), 726-734.

[8] A. Djemel, R.J.Tarento, J. Castaing, Y. Marfaing and A. Nouiri, Study of electronic surface properties of GaAs in cathodoluminescence experiments, *Phys. Stat. Sol. (a)*, 168, (1998) 425-430.

[9] A. Djemel, A. Nouiri, S. Kouissa, and R. J. Tarrento, Cathodoluminescence calculation of GaAs. Surface analysis and comparison, *Phys. Stat. Sol. (a)*, 191, (2002), 223-229.

[10] D. Kenieche and K.Guergouri, Theoretical calculation of cathodoluminescence: Infuence of surface and bulk parameters on the depletion region of p-type CdTe, *Mod. Phys. Lett. B* , 30, (2016),1650057.

[11] D. Kenieche and K. Guergouri, Theoretical Investigation of the Effect of the Surface Parameters on Cathodoluminescence Signal, *J. Mat. Sci. Eng*., 5, (2011), 473-477.

[12] C. J. Wu, D.B. Wittry, Investigation of minority-carrier diffusion lengths by electron bombardment of schottky barriers, *J. Appl. Phys.,* 49, (1978), 2827-2836.

[13] K. Kanaya , S. Okayama, Penetration and energy-loss theory of electrons in solid targets, *J. Phys. D : Appl. Phys*., 5, (1972),43-58,.

[14] W. Hergert and L. Pesemann, Theoretical study of the information depth of the cathodoluminescence signal in semiconductor materials, *Phys. Stat. Sol. a* 85, (1984), 641-648.

[15] B. G. Yacobi et D. B. Holt, *Cathodoluminescence Microscopy of Inorganic Solids*, Ed. Pelenum Press, New York and London, (1990), 68.