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Characterization of semi-insulating GaAs:Cr by means of DC-CPM technique

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Abstract - *In the present paper, constant photocurrent method, 'CPM' is used to determine the defects distribution from the optical absorption spectra of semi-insulating Cr-doped GaAs. By using the derivative method, we have extracted the distribution of the density of states DOS close to valence band edge E_v from the measured optical absorption spectrum. We have also developed a computer code program dc-CPM which have been used to compute the total absorption spectrum and their components using a model density of states inferred from two complementary techniques: constant photocurrent method, 'CPM' and transient photocurrent 'TPC'. It is found that by combination of the two measurement techniques 'CPM' and 'TPC', and the two absorption spectra components α_n and α_p, we are able to have a full reconstruction of the density of states distribution below and above the Fermi level for such materials.*

Résumé - *Dans ce présent travail, on a déterminé la distribution énergétique des défauts du GaAs:Cr en utilisant son spectre d'absorption optique mesuré par la technique du photo courant constant, 'CPM'. Ainsi et par dérivation du spectre d'absorption optique mesuré, on a pu déterminer la densité d'états électronique DOS près de la bande de valence E_v. On a aussi développé un programme pour modéliser la technique dc-CPM en régime continu. Un modèle de densité d'états a été proposé en se basant sur deux techniques complémentaires, la technique 'CPM' et la technique du photo-courant transitoire 'TPC', pour calculer le coefficient d'absorption optique total, ainsi que les deux coefficients d'absorption optique α_n et α_p,dues aux électrons et aux trous respectivement. On a trouvé que par la combinaison des deux techniques CPM et TPC d'un coté, et les deux spectres d'absorption α_n et α_p, d'un autre coté, on aboutit à déterminer la distribution énergétique de la densité d'état électronique sur tout le gap au-dessous et au-dessus de niveau de Fermi pour ce type de matériaux.*

Keywords: Constant photocurrent method, Transient photocurrent, Optical absorption spectrum, Gallium arsenide, Defect states.

1. INTRODUCTION

Gallium arsenide GaAs material is widely used in the semiconductor industry due to its wider direct band gap energy E_g and higher electron mobility μ_n (E_g = 1.42 eV and μ_n = 8500 $cm^2V^{-1}s^{-1}$) compared to crystalline silicon (E_g = 1.12eV and μ_n = 1350 $cm^2V^{-1}s^{-1}$). These properties make this material very useful for infrared light emitting and laser diodes manufacturing.

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GaAs can be doped with Chromium (Cr) in order to obtain a semi-insulating gallium arsenide (SI-GaAs:Cr) substrate as silicon dioxide. Chromium behaves as an acceptor with an impurity level close to the centre of the energy gap [1-3].

Defect levels in semiconductor band gaps determine the electrical and optical properties devices. These properties are determined by the relative position of the level and the capture cross section of the carriers. The defect levels can capture minority, majority carriers or both carriers for the deep states and they act, in this case, as recombination centres.

Usually, capture and release of majority and minority carriers at defect levels phenomena in semiconductors materials is characterised by deep level transient spectroscopy, 'DLTS' [4] and minority carrier transient spectroscopy, 'MCTS' [5]. For semi-insulating (SI) crystals like GaAs and amorphous materials like a-Si:H other techniques should be used such as CPM [6-8], TPC [9] and modulated photoconductivity MPC [10, 11].

The purpose of this present work is to investigate the shallow and deep defect levels distribution in semi-insulating GaAs:Cr by constant photocurrent method by combination of measurement and simulation results.

2. THEORY AND SIMULATIONS

Photocurrent techniques detect optically induced transitions between localised (defect) levels in the band-gap and extended levels in the bands, which generates free carriers. This should allow one to determine, by appropriate spectroscopy methods, the density and energy position of the defect states within the forbidden optical gap.

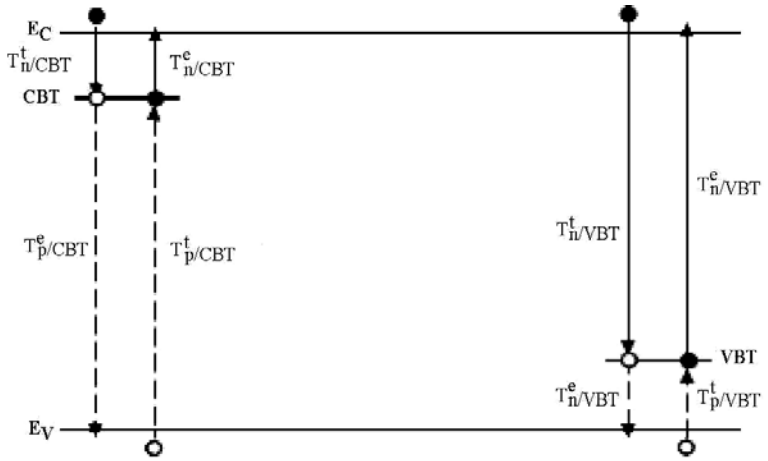
The CPM was first introduced by Vanecek *et al.* [12, 13] with the basic idea to adjust the photon flux $\phi(h\nu)$ in such a manner that the photocurrent remains constant for all incident photon energies $h\tilde{\nu}$ Under these conditions, one ensures that the occupation of the electronic states, the concentration of the photo-generated carriers and the product $(\mu\tau)$ remain constant for all used wavelengths λ. These are the conditions of validity of the CPM method. If the photocurrent is constant during the measurements, the inverse number of the incident photons is proportional to the absorption coefficient $\alpha(h\nu)$.

$$\alpha(h\nu).\phi(h\nu) = \text{Cte} \quad \Rightarrow \quad \alpha(h\nu) \propto \frac{1}{\phi(h\nu)} \tag{1}$$

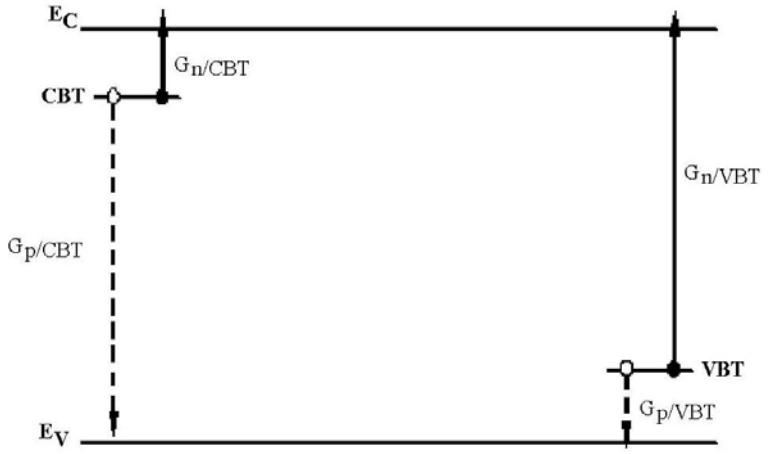
Figure 1 illustrates the thermal and optical carrier transitions for the CPM for a uniform sub-gap illumination. While single level representation appears in the illustration, the DOS is energy-distributed. At room temperature, photoconduction is carried out by free carriers, and so the only transitions taken into account are those between localised states in the gap and extended states in the bands. In addition, because of their small probabilities, band-to-band transitions are ignored.

The thermal transition rates T have the following significance:

- $T^{t(e)}_{n(p)/CBT(VBT)}(E)$: Rates of trapping (emission) of electron (hole) into (from) a level E at the conduction band tail (valence band tail).



a- Thermal transitions



b- Optical transitions

Fig. 1: Carrier transitions involved in the CPM simulation
o: Hole, ----- : Hole transitions
●: Electron, — : Electron transitions

The trapping rate is a function of free $n(p)$ and trapped $n_t(p_t)$ carrier densities following the relation

$$T^t_{n(p)}(E) = C_{n(p)}\, n(p)\left[D(E) - n_t(p_t)\right] \tag{2}$$

where $D(E)$ is the total DOS at level E and $C_{n(p)}$ is the capture coefficient of the trapping state.

Similarly, the emission rate is a function of trapped $n_t(p_t)$ carrier densities following the relation:

$$T^{e}_{n(p)}(E) = C_{n(p)} D_{CB(VB)} n_t(p_t).\exp\left(-\left|E - E_{CB(VB)}\right| / \left(k_B T\right)\right) \quad (3)$$

where $D_{CB(VB)}$ is the effective DOS at the conduction (valence) mobility edge $E_{CB(VB)}$ (k_B is Boltzmann constant and T the temperature).

The optical generation rates G have the following significance:

- $G_{n(p)/VBT(CBT)}(E)$: Rates of electron (hole) generation from a level E at the valence band tail (conduction band tail).

The optical generation rate is function of the free and trapped carrier densities following the equation:

$$G_{n(p)}(E, h\nu) = \phi \times \left(\frac{K}{h\nu}\right) \times \left(D_{CB(VB)} - n(p)\right) \times n_t(D)(E) \quad (4)$$

where ϕ is the incident photon flux and $K = 4.34\times10^{-38}\ cm^5\,eV^2$ is a constant proportional to the momentum matrix element.

For the steady-state regime, we have to solve the following equations:

- **Neutrality equation**

$$n_{dc} + \int_{E_v}^{E_c} n_t^{dc}(E) - p - \int_{E_v}^{E_c} n_t^{dc}(E) - Dop = 0 \quad (5)$$

Where Dop is ionised dopant charge density.

- **Continuity equation for free charges** n_{dc} and p_{dc}

$$\begin{aligned} &\frac{dn_{dc}(t)}{dt} = 0 \\ &\int_{E_V}^{E_C}\left(T^{e}_{n/CBT} + T^{e}_{n/CBT} - T^{t}_{n/VBT} - T^{t}_{n/VBT}\right).dE \\ &\quad + \int_{E_V}^{E_C} G^{dc}_{n/VBT}.dE + \int_{E_V}^{E_C} G^{dc}_{n/CBT}.dE = 0 \end{aligned} \quad (6)$$

$$\begin{aligned} &\frac{dp_{dc}(t)}{dt} = 0 \\ &\int_{E_V}^{E_C}\left(T^{e}_{p/CBT} + T^{e}_{p/VBT} - T^{t}_{p/CBT} - T^{t}_{p/VBT}\right).dE \\ &\quad + \int_{E_V}^{E_C} G^{dc}_{p/CBT}.dE + \int_{E_V}^{E_C} G^{dc}_{p/CBT}.dE = 0 \end{aligned} \quad (7)$$

- **Rate equation for trapped carriers** n_t and p_t

$$\frac{dn_t^{dc}(E, t)}{dt} = 0 \qquad \Rightarrow$$

$$T^{t}_{n/CBT} - T^{e}_{n/CBT} + T^{e}_{p/CBT} - T^{t}_{p/CBT} + G^{dc}_{p/CBT} - G^{dc}_{n/CBT} = 0 \qquad (8)$$

$$\frac{dp_t^{dc}(E,t)}{dt} = 0 \qquad \Rightarrow$$

$$T^{t}_{p/VBT} - T^{e}_{p/VBT} + T^{e}_{n/VBT} - T^{t}_{n/VBT} + G^{dc}_{n/VBT} - G^{dc}_{p/CBT} = 0 \qquad (9)$$

To solve the dc-CPM equations (5) to (9), we divide the energy gap into N closely spaced energy levels E_i, including the band edges $E_V = E_1$ and $E_C = E_N$.

In modeling coplanar samples, it is a common practice to assume uniform electric field, perfect ohmic contacts, and to neglect any transport driven by free-carrier diffusion. Under these assumptions, the continuity equation for holes is automatically satisfied when the continuity equation for electrons and the charge neutrality condition are fulfilled. We have developed a computer code to solve the system of equations (5) to (9) using appropriate numerical techniques. All the thermal and optical transition rates $T^{dc}(E)$ and $G^{dc}(E, h\nu)$ can be deduced from equations (2), (3) and (4) as follow:

$$T^{t}_{n(p)}(E) = C_{n(p)} \times n_{dc}(p_{pc}) \times \left[D(E) - n_t^{dc}(p_t^{dc}) \right] \qquad (10)$$

$$T^{e}_{n(p)}(E) = C_{n(p)} \times D_{CB(VB)} \times n_t^{dc}(p_t^{dc}) \times \exp\left(- \left| E - E_{CB(VB)} \right| / (k_B T) \right) \qquad (11)$$

$$G^{dc}_{n(p)}(E, h\nu) = \phi_{dc} \times \left(\frac{K}{h\nu} \right) \times \left(D_{CB(VB)} - n_{dc}(p_{dc}) \right) \times n_t^{dc}(D)(E) \qquad (12)$$

As required by the CPM experiment, the photon energy $h\nu$ is varied and the dc photon flux magnitude ϕ_{dc} is adjusted to keep the magnitude of the dc-photoconductivity $q(\mu_n n_{dc} + \mu_p p_{dc})$, constant over the whole $h\nu$ range. The single transition dc absorption coefficient is then deduced from equation (12) as:

$$\alpha^{dc}_{n(p)}(E_i, h\nu) = \frac{G_{n(p)}(E_i, h\nu)}{\phi_{dc}} = \left(\frac{K}{h\nu} \right) \times D_{CB(VB)}\, n_t^{dc}(E_i) \times \left[D(E_i) \right] \qquad (13)$$

and the total absorption coefficient as:

$$\alpha^{dc}_{n(p)}(h\nu) = \sum_i \alpha^{dc}_{n(p)}(E_i, h\nu) \qquad (14)$$

The DOS distribution is calculated from the absorption coefficient, after Pierz *at al.* [15], using the derivative:

$$g(E) = \frac{1}{K g(E_V)} \left[\frac{d\left(h\nu\, \alpha^{dc}_{n(p)}(h\nu) \right)}{d(h\nu)} \right]_{h\nu = E_C - E} \qquad (15)$$

3. EXPERIMENTAL DETAILS

The GaAs:Cr 1713 sample was prepared at Ruđer Bošković Institute Division of Materials Physics, Zagreb, Croatia. The 1713 sample was part of a semi-insulating GaAs chromium doped wafer (GaAs:Cr) of 400 μm thickness. It was cut from the ingots grown in the <100> direction by the liquid encapsulated Czochralski (LEC) method under B_2O_3 encapsulation. The chromium concentration was 1.5 x 10^{16} cm^{-3}. Arrays of coplanar ohmic electrodes were deposited on the polished surface of the wafers with a gap of 0.8 mm between electrodes. Single chips of 4 x 9 mm^2 in area were cut from the wafers and mounted in the sample holders of cryostats.

The schematic of the CPM experiment which have been used in this work is shown in figure 2. A xenon lamp was used as a light source. The monochromator had a grating of 600 grooves/mm with a filter wheel were used for scanning wavelength. The dc-CPM current was measured by a picoammeter instead of a lock-in amplifier but the light intensity was monitored by the same lock-in method as in the case of ac-CPM.

In the CPM, absorption coefficients, $\alpha(h\nu)$, were obtained as the inverse of the incident photon number, $1/\phi_{ph}$, under a constant photocurrent, I_{ph}, by using conventional CPM assumptions.

Absolute CPM spectra were obtained by monitoring the transmitted photon flux following the procedures described by Vanecek *et al.* [12, 13]. Data were then calibrated by reference to optical transmission measurements, through the use of the Ritter-Weiser formula [14].

The DOS was obtained by differentiation of the absorption curve method described by Pierz *et al.* [15].

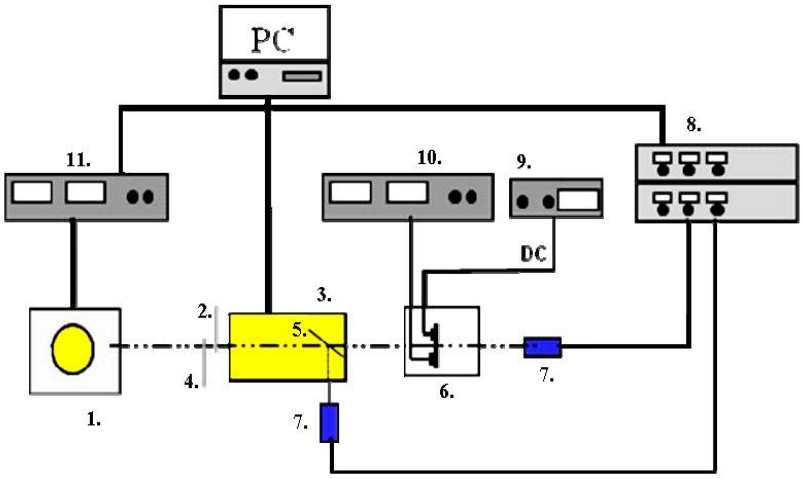
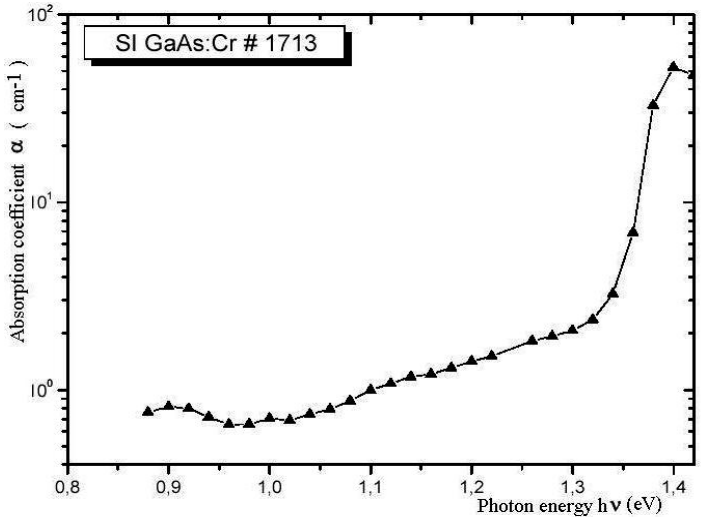


Fig. 2: DC-CPM set up

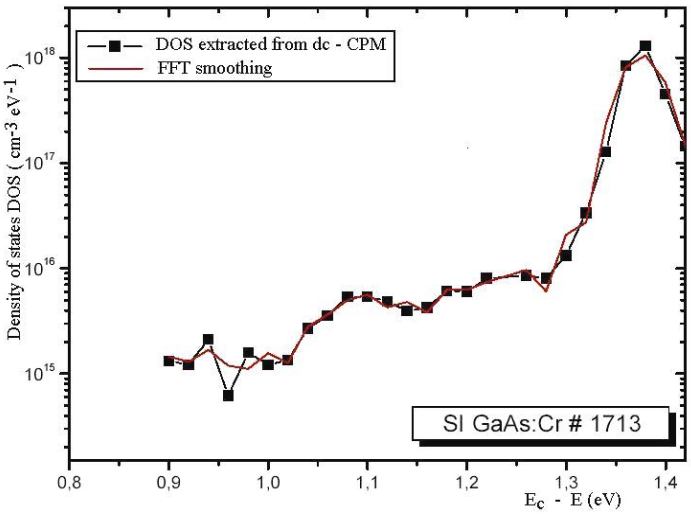
1. W-halogen lamp; 2.Optical chopper; 3. Monochromator; 4. Filters wheel
5. Beam splitter; 6. Cryostat+ Sample; 7. Detectors; 8. Lock-in amplifier
9. Picoammeter; 10.Sample power supply; 11. Lamp power supply

4. RESULTS AND DISCUSSION

Figure 3-a show the measured Cr doped GaAs CPM spectrum. A rapid decrease in the absorption coefficient is observed at about 1.4eV which is the band edge for this material. Figure 3-b show the density of states distribution of occupied states close to valence band edge derived from figure 3-a using the derivative method of Pierz *et al.* [15].



(a)



(b)

Fig. 3: dc-CPM spectrum (a) and the corresponding density of states distribution (b) for SI GaAs:Cr # 1713 sample

A density of states distribution model for the semi-insulating Cr-doped GaAs is introduced and shown in figure 4. The introduced density of states consists of two parts:

(i) the lower part close to conduction band edge is derived from transient photocurrent measurement TPC, [2], high resolution photo induced transient spectroscopy HRPITS and modulated photocurrent measurements MPC [3],

(ii) while the upper part near the valence band edge is derived from CPM measurement as shown in figure 3-(b).

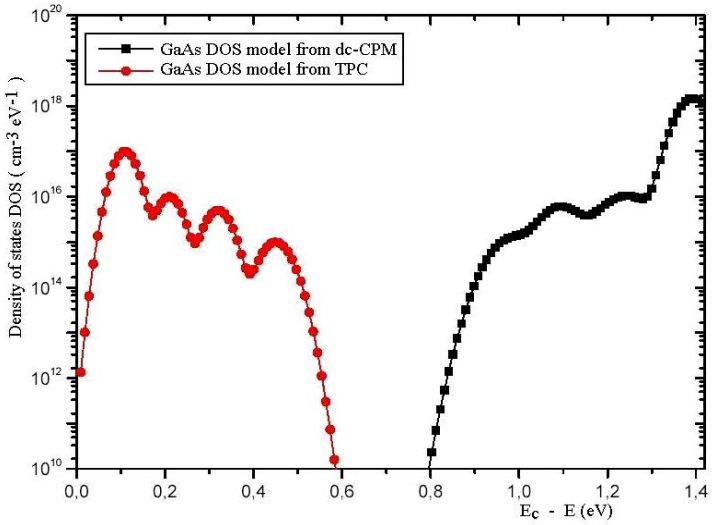


Fig. 4: Semi-insulating Cr-doped GaAs density of states distribution model used for CPM numerical modelling

The most important parameters used for this density of states distribution are summarized in **Table 1**.

Table 1: Density of states parameters used in optical absorption spectrum modelling of SI GaAs:Cr

Electron mobility	$\mu_n = 4400\ cm^2V^{-1}s^{-1}$
Hole mobility	$\mu_p = 100\ cm^2V^{-1}s^{-1}$
Density of states at the mobility edge E_c	$N_c = 4.7 \times 10^{17}\ cm^{-3}$
Density of states at the mobility edge E_v	$N_v = 7 \times 10^{18}\ cm^{-3}$
Mobility Gap	$E_g = 1.42$ eV
Temperature	$T = 300°K$
Fermi level position E_F^*	0.75 eV

*E_F is calculated from the charge neutrality condition

Using the SI GaAs:Cr DOS model, we have computed by our CPM program code the total absorption coefficient α_{dc-tot} and their components α_{dc-n} and α_{dc-p}, corresponding to optical transitions associated with free electron and free hole creation respectively. These absorption spectra are used to infer the density of states over the energy gap near band edge and close to mid-gap.

Figure 5 and 6 show the obtained results. As we can see the actual DOS is well fitted over a large region of the band gap of the semi-insulating Cr-doped GaAs.

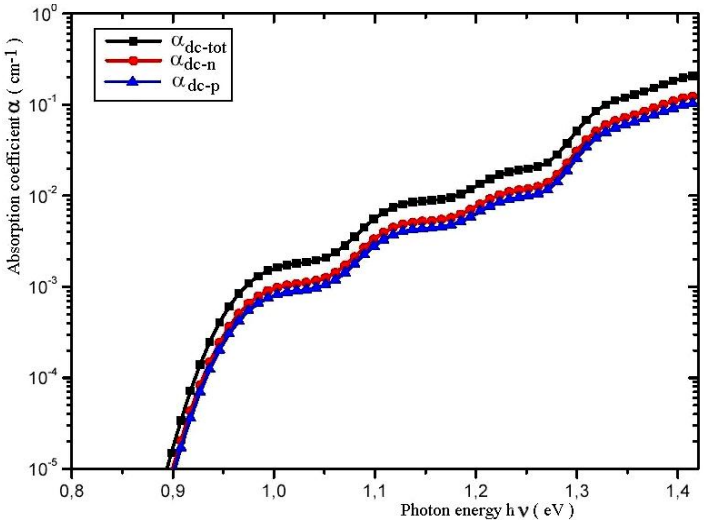


Fig. 5: Simulated dc-CPM spectra for Cr doped GaAs using the DOS of figure 4:
(■) total absorption spectrum α_{dc-tot} (hν)
(●) Simulated dc-CPM electron absorption spectrum α_{dc-n} (hν)
(▲) Simulated dc-CPM hole absorption spectrum α_{dc-p} (hν).

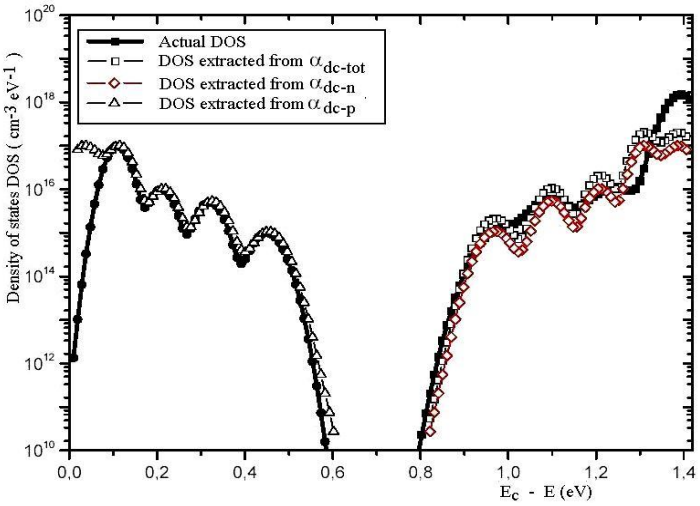


Fig. 6: Reconstructed density of states from absorption spectra of figure 5

5. CONCLUSION

In conclusion, the measurement results have shown that the absolute CPM technique is applicable to non-silicon materials such as Gallium Arsenide and to any photoconductive materials. While, and on the other hand, the simulation results have allowed us the determination of the distribution of defects below and above the Fermi level from $\alpha_{dc-n}(h\nu)$ and $\alpha_{dc-p}(h\nu)$ absorption coefficients. It is also found that by combination of the two well known measurement methods CPM and TPC, and the two experimentally inaccessible optical absorption coefficients components $\alpha_n(h\nu)$ and $\alpha_p(h\nu)$, we are able to have a full reconstruction of the occupied and unoccupied density of states distribution for such materials.

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