SIMULATION OF THE PRE- AND POST-TRANSIT TIME OF FLIGHT METHODS IN AMORPHOUS SILICON-LIKE. N^+-I-P^+ -CELLS

SIMULATION DES METHODES DE PRE- ET POST-TRANSIT DE LA TECHNIQUE TEMPS DE VOL POUR LES CELLULES N^+-I-P^+ EN MATERIAU DE TYPE a-Si:H.

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ABSTRACT

In this paper, we study, by numerical simulation, the Transient Photocurrent (TPC) resulting from the application of the 'Time Of Flight' (TOF) technique to a-Si:H n^+-i-p^+ cell by using a typical Density Of States (DOS) of amorphous silicon. The pre- and post-transit methods, currently used to probe the energy distribution of localised states, are then applied to reconstruct the proposed DOS from the simulated TPC. We demonstrate that the two methods of reconstruction are complementary and provide an efficient tool of determining the transit time.

RESUME

Dans cet article, nous étudions, par simulation numérique, le photocourant transitoire (PCT) résultant de l'application de la technique 'temps de vol' (TOF) à une cellule n^+-i-p^+ en a-Si:H en utilisant une densité des états (DOS) typique au silicium amorphe. Les deux méthodes de pré et post-transit, couramment utilisées pour déterminer la distribution énergétique des états localisés dans le gap, sont ensuite appliquées au PCT simulé pour reconstruire la DOS proposée. On démontre que les deux méthodes de reconstitution sont complémentaires et fournissent un moyen de détermination du temps de transit.

1. INTRODUCTION

The degradation of a-Si:H solar cells presents a serious problem concerning their use in technological and commercial domain. To obtain a quality of a-Si:H more and more stable, several methods were developed. The TOF technique is one of the most used experiments for the opto-electric characterisation of a-Si:H solar cells. This technique uses, as a parameter, the transit time (or the flight time), t_T, required for the photo-generated charge to cross the sample after a rapid optical excitation of a reverse biased n-i-p diode [1, 2, 3]. In this paper, we present numerical simulation results of the TOF technique applied to the n^+-i-p^+ structure in the current mode. We examine the degree of reconstruction of the actual DOS proposed for the TPC simulation. We demonstrate that the pre- and post-transit methods, applied to the simulated TPC to reconstruct the DOS, are complementary and allow for the determination of the transit time t_T.

2. TOF TECHNIQUE

Fig. 1. depicts the principle of the TOF method. The a-Si:H-like sample consists of a n^+-i-p^+ structure with electrodes on either side.

First, the voltage pulse and, with a certain delay Δt, the short laser pulse of highly absorbed light are applied to the sample. Electron-hole pairs are then generated near the illuminated junction and separated by the applied electric field. This separation is such that the front electrode collects all charges of the same sign, while charges of the opposite sign cross the sample towards the other electrode. During the transient, the charge of the photogenerated carriers interacts with traps existing along the intrinsic region. Therefore, the measured TPC will give information on the localised states energy distribution of the material to be characterised.

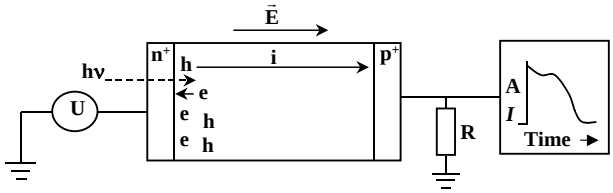

Figure 1. Schematic diagram of the TOF technique.

3. PRE AND POST-TRANSIT METHODS

Several spectroscopic methods have been put forward for the interpretation of TPC measurements in amorphous

semiconductors. In this paper, we emphasise on the pre- and post-transit methods [4].

The pre-transit method is applied to the TPC in the pre-transit region and probes states having release times shorter than t_T. This method is based on the multiple-trapping model developed by Tiedje and Rose [5], and Orenstein and Kastner [6]. It is assumed here that the density of states is distributed continuously and the carriers thermalise without loss by recombination or extraction after completion of transit. Thermalisation occurs such that, at a time t following the optical excitation, most of the carriers are concentrated in states close to a "thermalisation energy", E_{th}. For the case where transport occurs by holes, E_{th} is given by

$$E_{th} = E_v + kT\,ln(\nu t) \tag{1}$$

where ν is the attempt-to-escape frequency for the localised states, T is the temperature and k is Boltzmann's constant. This model allows the determination of the DOS, $g(E_{th})$, at energy E_{th} according to the following expression:

$$g(E_{th}) = \frac{C}{I(t).t} \tag{2}$$

where C is a constant.

The post-transit method, on the other hand is applied to the post-transit region of the TPC. In this case, the TPC is controlled by thermal emission of carriers that have been trapped in states having a release time longer than t_T. The DOS, $g(E_{th})$, is then determined by the expression:

$$g(E_{th}) = C'.I(t).t \tag{3}$$

4. TPC SIMULATION

Our sample consists of a 0.5µm a-Si:H n^+-i-p^+ cell, where the front illuminated side is the n region which is positively polarised. It means that we study transport of holes. For computation of the TPC, we use Poisson's equation (eq (4)), the continuity equations (eqs (5) and (6)) and the multi-trapping equations (eqs (7) and (8)).

$$\Delta\psi(x,t) = -\frac{q}{\varepsilon\varepsilon_o}\left[p(x,t) - n(x,t) + \sum_i p_t(x,E_i,t) - \sum_i n_t(x,E_i,t) \right] \tag{4}$$

$\psi(x,t)$ is the potential through the sample. p(x,t) and n(x,t) are the free holes and electrons concentrations. $p_t(x,E_i,t)$ and $n_t(x,E_i,t)$ are the hole and electron concentrations trapped by the i^{th} energy level E_i of the sub-divided gap.

$$\frac{\partial p(x,t)}{\partial t} = -\frac{1}{q}\frac{\partial J_p}{\partial x} - \sum_i T_p^c(x,E_i,t) - \sum_i T_p^v(x,E_i,t) + G(x,t) \tag{5}$$

$$\frac{\partial n(x,t)}{\partial t} = \frac{1}{q}\frac{\partial J_n}{\partial x} - \sum_i T_n^c(x,E_i,t) - \sum_i T_n^v(x,E_i,t) + G(x,t) \tag{6}$$

$$\frac{\partial p_t(x,E_i,t)}{\partial t} = T_p^v(x,E_i,t) - T_n^v(x,E_i,t) \tag{7}$$

$$\frac{\partial n_t(x,E_i,t)}{\partial t} = T_n^c(x,E_i,t) - T_p^c(x,E_i,t) \tag{8}$$

G (x,t) refers to the generation rate.

The terms $T_p^v(x,E_i,t), T_n^v(x,E_i,t)$ refer, respectively, to the net hole and electron trapping rates at the position x, in the instant t, at a level E_i of the valence band tail.

We have

$$T_p^v(x,E_i,t) = C_p^v\,p(x,t)\left[N_t^v(E_i) - p_t(x,E_i,t)\right] - e_p^v(E_i)\,p_t(x,E_i,t) \tag{9}$$

$$T_n^v(x,E_i,t) = C_n^v\,n(x,t)\,p_t(x,E_i,t) - e_n^v(E_i)\left[N_t^v(E_i) - p_t(x,E_i,t)\right] \tag{10}$$

where C_p^v, C_n^v are capture coefficients for holes and electrons and e_p^v, e_n^v are emission probabilities for the valence band tail states given by

$$e_p^v(E_i) = C_p^v N_v exp\left(\frac{E_v - E_i}{kT}\right), \qquad e_n^v(E_i) = C_n^v N_c exp\left(\frac{E_i - E_c}{kT}\right) \tag{11}$$

$T_p^c(x,E_i,t), T_n^c(x,E_i,t)$ are, respectively, the net hole and electron trapping rates at the position x, in the instant t, at a level E_i of the conduction band tail.

$$T_p^c(x,E_i,t) = C_p^c\ p(x,t)\ n_t(x,E_i,t) - \\ - e_p^c(E_i)\left[N_t^c(E_i) - n_t(x,E_i,t)\right] \quad (12)$$

$$T_n^c(x,E_i,t) = C_n^c\ n(x,t)\left[N_t^c(E_i) - n_t(x,E_i,t)\right] - \\ - e_n^c(E_i)\ n_t(x,E_i,t) \quad (13)$$

C_p^c, C_n^c are capture coefficients for holes and electrons and e_p^c, e_n^c are emission probabilities for the conduction band tail states given by

$$e_p^c(E_i) = C_p^c N_V exp\left(\frac{E_V - E_i}{kT}\right), \\ e_n^c(E_i) = C_n^c N_c exp\left(\frac{E_i - E_c}{kT}\right) \quad (14)$$

The total current density (J) is given by the sum of hole (J_p), electron (J_n) and displacement (J_d) currents.

$$J(t) = \frac{1}{d}\int_0^d \left(J_p(x,t) + J_n(x,t)\right)dx + \frac{\varepsilon\varepsilon_O}{d}\int_0^d \frac{\partial\zeta(x,t)}{\partial t}dx \quad (15)$$

where

$$J_p(x,t) = q\,\mu_p\left[p(x,t)\,\zeta(x,t) - \frac{kT}{q}\frac{\partial p(x,t)}{\partial x}\right] \quad (16)$$

$$J_n(x,t) = q\,\mu_n\left[n(x,t)\,\zeta(x,t) + \frac{kT}{q}\frac{\partial n(x,t)}{\partial x}\right] \quad (17)$$

d is the sample thickness, $\varepsilon\varepsilon_O$ the permittivity and $\zeta(x,t)$ the electric field distribution.

As initial conditions, we assume a homogeneous electric field distribution along the sample, the instantaneous generation of electron-hole pairs according to the exponential law given by the absorption coefficient α, and the thermal equilibrium for the initial occupation of the band tails. Boundary conditions are given by $\psi(0,t) = U_O + U_i$ and $\psi(d,t) = 0$, where zero and d are the positions of the front and rear electrodes respectively, U_O is the applied voltage and U_i is the built-in voltage.

The voltage across the sample is assumed to be constant at all times and $\int_0^d \zeta(x,t) = U_O + U_i = \text{constant}$, so the transient current density J(t) can be calculated simply from the hole and electron current.

Equilibrium is assumed for the region adjacent to the metal end-contacts, so that the relation $n\,p = n_i^2$ is verified at these points (n_i is the intrinsic concentration).

The proposed DOS (for the valence band tail) used in this simulation is shown in Fig.2.

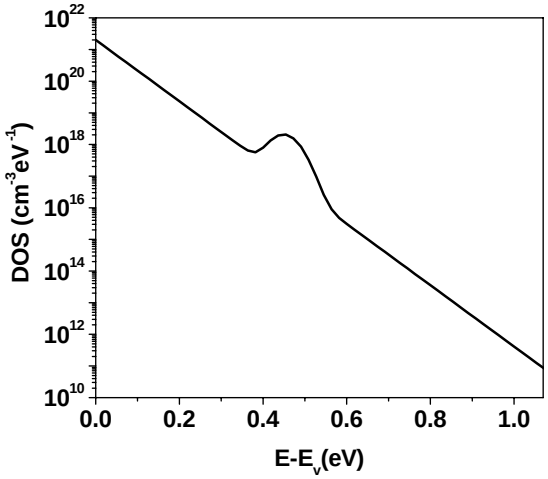

Figure 2 : Proposed DOS for the valence band tail.

It is composed of an exponential band tail (characteristic temperature $T_V = 520°\text{K}$), plus a Gaussian distribution of deeper states (central energy $E_O = 0.45\,\text{eV}$, characteristic temperature $T_O = 500°\text{K}$):

$$g(E) = G_V exp\left(\frac{E_V - E}{kT_V}\right) + \frac{G_V}{10^3} exp\left[-\left(\frac{E - E_O}{kT_O}\right)^2\right] \quad (18)$$

where $G_V = 2\times10^{21}\,\text{cm}^{-3}\text{eV}^{-1}$ and $E_V = 0\,\text{eV}$ (all energy values are measured upwards from the valence band mobility edge, E_V).

The system of equations describing charge transport has been solved using finite difference method. To simplify, we have considered only the one-dimensional case in which, the different variables are function of the spatial co-ordinate x and of the time t. [7, 8].

5. SIMULATION RESULTS

Fig.3 shows the simulated hole TPC under 2V reserve bias, with T=300°K and T_v=520°K. the photogenerated charge Q_0 is $6.3\text{x}10^{-7}\text{Ccm}^{-2}$ with $\alpha=6\text{x}10^5\text{cm}^{-1}$.

The curve shows a dispersive transport of holes through the intrinsic region. At very short times, lower than about 10^{-11} sec, the TPC is dominated by initial trapping of free carriers in the tails states, followed by the pre-transit thermalisation. After, the TPC decays according to the 'post-transit' regime defined above. The intersection point t_T, separating the tow regimes represents the transit time, we have $t_T \cong 10^{-7}$ sec .

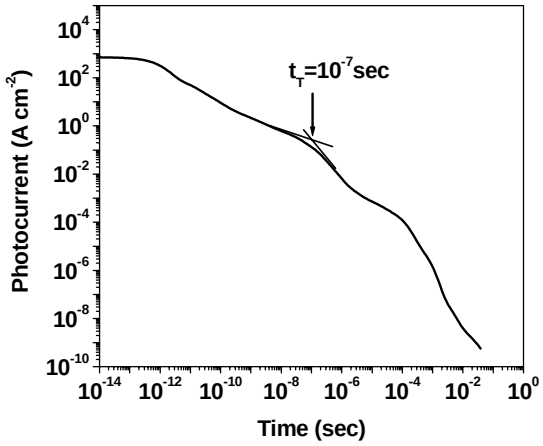

Figure 3: Simulated TPC for hole transport

Fig.4 presents the DOS reconstructed from the simulated TPC of Fig.3 using both the pre- and post-transit techniques.

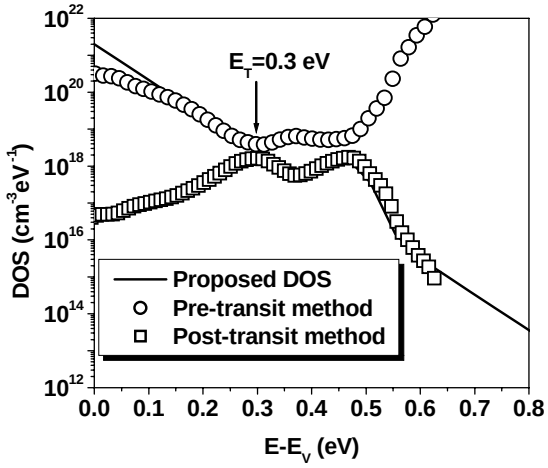

Figure 4: Reconstructed DOS using the pre and post-transit methods

According to this curve, we can notice that the reconstruction gives a result that agrees reasonably well with the proposed DOS over a wide energy range. Besides, the two methods are complementary and the transit time t_T can be calculated from the energy level E_T using the thermalisation relation $E_T = E_V + kT\,ln(\nu t_T)$, E_T, being the level above (below) which the DOS calculated by the pre- (post-) transit method begins to diverge.

The calculated t_T value is shown in Table 1 together with the t_T value deduced from the TPC.

Table 1: Calculation results of t_T.

DOS		TPC
E_T (eV)	t_T (sec)	t_T (sec)
0.3	1.084×10^{-7}	10^{-7}

the value of t_T calculated from E_T is close to that determined from the TPC within a precision of about 8.12%.

CONCLUSION

In this work, we have simulated transient photoresponse of a n^+-i-p^+ structure obtained by the TOF technique. We have demonstrated that the transit time can be determined from the DOS obtained by application of both the pre- and post-tarnsit TOF methods.

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