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Time photocurrent response and the density of localised states in disordered semiconductors

A. Merazga*, M. Herbane

Department of Physics, Faculty of Science, King Khaled University, PO Box 9004, Abha, Saudi Arabia

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Abstract

The Time Photocurrent Response (TPR) of a disordered semiconductor to a step-like super-gap excitation is examined by numerical simulation under the assumption of one carrier (electron) multiple-trapping and transport, using exponential and featured model density of localised states $g(E)$. A 'plateau' feature in the TPR, followed by a rapid increase and a subsequent turn over to a steady state level, is observed. This is correlated to the Gaussian 'bump' feature of $g(E)$ by studying the relative change with time of the net trapping and recombination rates. The simulation results are validated for a typical photosensitive disordered semiconductor, the a-SiH.

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1. Introduction

Photocurrent techniques with static and/or dynamic photoexcitation have been extensively used to characterise photosensitive semiconductors, such as for example the steady state photocurrent [1], the transient photocurrent [2,3], the modulated photocurrent [4,5] and the constant photocurrent [6]. The most important characteristic to determine by these techniques in such semiconductors is the energy distribution of the density of localised states $g(E)$, as this reflects defect states that can obscure their photocurrent response and degrade the performance of their related optoelectronic devices.

The transient photocurrent (TPC), among these techniques, is probably the most suitable direct method to reveal the $g(E)$ distribution in disordered semiconductors. In this method, the TPC decay following the very brief light pulse shows features that are images of features in the $g(E)$ distribution. Quantitative correlation between the TPC decay and the $g(E)$ distribution, based on multiple-trapping (MT) and transport analysis, has led to a detailed spectroscopy method to determine $g(E)$ from the TPC [7].

In the TPC, the photocurrent initiates at a maximum due to the light-pulsed free carrier density and decays via MT and recombination to the thermal equilibrium dark current. The question addressed in the present work concerns the inverse trend. That is the Time Photocurrent Response (TPR) to a step-like super-gap excitation where the photocurrent initiates at the thermal equilibrium dark current and rises via MT and recombination at constant photo-generation rate to approach a steady state level. We consider exponential and featured model $g(E)$ distributions and present an attempt to correlate the TPR to $g(E)$ by studying the relative change with time of the net trapping and recombination rates. We then present an experimental TPR result at $T = 300$ K for a typical photosensitive disordered semiconductor, the a-Si:H.

2. TPR simulation

Assuming one carrier (electron) multiple-trapping and transport, the numerical simulation of the TPR in a disordered semiconductor consists of solving the system of the m rate equations for free $n(t)$ and trapped $n_i(t)$ electron densities:

$$\frac{\mathrm{d}n(t)}{\mathrm{d}t} = -\sum_{i=2}^{m} \frac{\mathrm{d}n_i(t)}{\mathrm{d}t} - \omega_R n(t) + G(t) \quad (1)$$

* Corresponding author.
E-mail address: aamerazga@kku.edu.sa (A. Merazga).

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$$\frac{dn_i(t)}{dt} = -\omega_{ei} n_i(t) + \omega_{ti} n(t) \quad (i = 2, 3, \ldots, m) \tag{2}$$

where the ω-frequency factors are:

– $\omega_R = 1/\tau_R$: Recombination frequency,
– $\omega_{ei} = \nu \exp[(E_i - E_c)/kT]$: Emission frequency,
– $\omega_{ti}(t) = C_n[N_{ti} - n_i(t)] \sim C_n N_{ti}$: Trapping frequency,

C_n is the capture coefficient and $\nu = N_c \cdot C_n$ the attempt-to-escape-frequency, with N_c the effective density of states at the mobility edge E_c. k is the Boltzmann constant. The energy range above the Fermi level E_F is divided into a large number m of closely and uniformly spaced energy levels E_i ($i = 2, \ldots, m$), including the Fermi level $E_m = E_F$, to represent an approximation of the continuum of localized states. In this division, the mobility edge E_c of the extended states takes the first level $E_1 = E_c$ and the summation in Eq. (1) should then cover the $m - 1$ levels E_i ($i = 2, \ldots, m$) of localized state. $N_{ti} = g(E_i)dE(\text{cm}^{-3})$ is the density of states at level E_i, with dE the uniform energy step. The recombination is assumed to be monomolecular with a characteristic lifetime τ_R. The time function of the generation rate is defined by a step function of height $G_0(\text{cm}^{-3}\ \text{s}^{-1})$ starting at the time t_0:

$$G(t) = \begin{bmatrix} G_0 & \text{for } t > t_0 \\ 0 & \text{for } t < t_0 \end{bmatrix}. \tag{3}$$

The initial conditions are set at t_0 prior to excitation, where thermal equilibrium conditions of zero excess free and trapped electron densities exist. This will result in a TPR rising from zero photocurrent to a steady state level and the features observed in the TPR must reflect features in the $g(E)$ distribution.

Fig. 1 shows a simulated TPR at 300 K with $G_0 = 10^{20}\ \text{cm}^{-3}\ \text{s}^{-1}$ over the time range from 10 ns to 10 ms. The model $g(E)$ distribution used here is shown in Fig. 2 (thin solid curve). This is composed of an exponential conduction band tail of width E_0 with $G_c = g(E_c)$, and a Gaussian defect states distribution of width E_d, peaking at the energy level E_m below E_c with a maximum G_d:

$$g(E) = G_c \exp\left(\frac{E - E_c}{E_0}\right) + G_d \exp\left[-\left(\frac{E - E_m}{E_d}\right)^2\right]. \tag{4}$$

The simulation parameters including the constants of $g(E)$ in Eq. (4) are indicated in Table 1.

Table 1
Simulation parameters

Parameter	Unit	Value
C_n	$\text{cm}^3\ \text{s}^{-1}$	10^{-8}
N_c	cm^{-3}	10^{20}
E_F	eV	−0.75
G_c	$\text{cm}^{-3}\ \text{eV}^{-1}$	10^{22}
G_d	$\text{cm}^{-3}\ \text{eV}^{-1}$	10^{16}
E_0	meV	25
E_d	meV	100
E_m	eV	−0.55
τ_R	s	10^{-5}

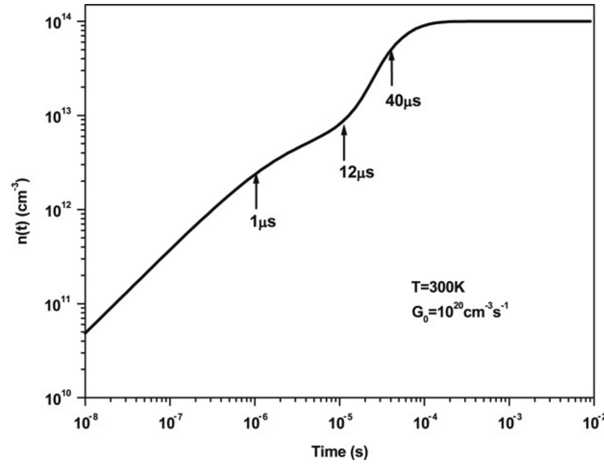

Fig. 1. Simulated TPR at 300 K with $G_0 = 10^{20}\ \text{cm}^{-3}\ \text{s}^{-1}$. The model $g(E)$ of the disordered semiconductor used for the TPR simulation is shown in Fig. 2 (thin solid line).

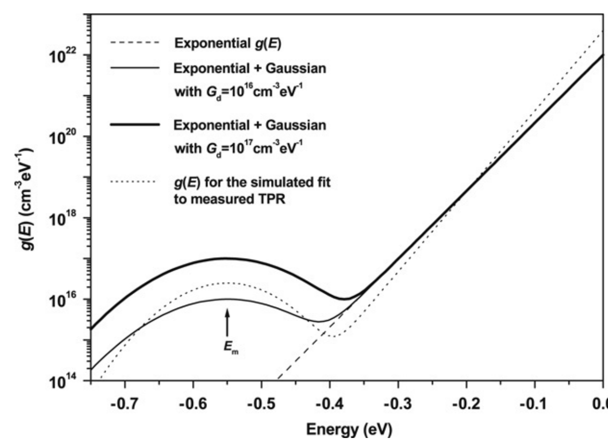

Fig. 2. Model density of states distributions $g(E)$ for TPR simulations: - - -: Exponential $g(E)$; –: Featured $g(E)$ by adding a Gaussian distribution with the maximum $G_d = 10^{16}\ \text{cm}^{-3}\ \text{eV}^{-1}$; **–**: Featured $g(E)$ by adding a Gaussian distribution with the maximum $G_d = 10^{17}\ \text{cm}^{-3}\ \text{eV}^{-1}$; ….: $g(E)$ distribution used for simulated TPR fit to the measured TPR.

A remarkable 'plateau' feature appears at about 1 μs and ends at about 12 μs when the TPR increases more rapidly until about 40 μs. Then the TPR turns over to level out for a steady state. To correlate this feature to the $g(E)$ distribution, we present, in Fig. 3, the graphs of two other simulated TPR: one (dashed curve) for an entirely exponential $g(E)$ ($G_d = 0\ \text{cm}^{-3}\ \text{eV}^{-1}$) and another (thick solid curve) for $g(E)$ with a higher Gaussian distribution ($G_d = 10^{17}\ \text{cm}^{-3}\ \text{eV}^{-1}$). The exponential and featured ($G_d = 10^{17}\ \text{cm}^{-3}\ \text{eV}^{-1}$)$g(E)$ distributions are shown in Fig. 2 by the dashed and thick solid curves respectively.

The TPR corresponding to the simple exponential $g(E)$ shows no such a 'plateau' feature, while the TPR corresponding to $g(E)$ with increased G_d to $10^{17}\ \text{cm}^{-3}\ \text{eV}^{-1}$ shows a more pronounced feature. Therefore, we conclude that the 'plateau' feature of the TPR is qualitatively correlated to the Gaussian 'bump' feature in the $g(E)$ distribution.

This correlation must be assured via the MT process occurring in parallel with the generation and recombination