SIMULATION STUDY OF THE PHOTOTRANSPORT IN AMORPHOUS SEMICONDUCTORS FROM TIME-OF-FLIGHT PHOTOCURRENT ANALYSIS

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Abstract

Time -of -flight transient photocurrent has been numerically analyzed. It is shown that the charge –carrier transit time can be determined in both non-dispersive and dispersive transport. It is also shown that the localized state distributions can be determined from the analysis of the photocurrent.

Introduction

The calculation of charge transport in amorphous materials with a spectrum of density of states in the mobility gap is well known to be complicated task widely discussed in literature [1-4]. During the past few years, there have been growing interests in obtaining exact solutions of transport equations. In particular exact solutions of the total carrier density equations in extended and localized states with various methods have been obtained by a number of authors [5,6]. Encouraged by the experimental realization of the transient photocurrents using the time of flight technique in different range of temperatures [3,7] we are interested in: (i) to improve the calculations of the electronic properties for the amorphous semiconductors, and (ii) to remove the divergence appears in the density of states distribution for amorphous selenium. The results obtained in this work show that the numerical model proposed is reliable for estimating the distribution of localized states from transient photocurrent measurements. These were obtained using the inverse Laplace transform

calculated numerically, using the method of Padé approximation [8]. We suggest that the proposed method can be used to confirm the shape of the density of states in the lower half of the gap in amorphous selenium which remains a controversial topic in the literature [9,10].

Theory of Laplace transforms method

The time of flight technique has been widely applied to a broad range of materials to determine, not only the drift mobility of the photoinjected charge carriers but also the distribution of traps, since the latter affects the magnitude of the instantaneous photocurrent. In the time-of-flight (TOF) experiment, a semiconductor is sandwiched between current-blocking contacts and a strongly absorbed light pulse creates free carriers just beyond one (semitransparent) contact. An electric field across the sandwich cell will then, depending on its polarity, drift either electrons or holes through the cell and cause a matching conduction current in the external circuit. Up to the TOF transit time , i.e. the time it takes for a representative set of the drifting carriers to reach the collection electrode, the transient current can be analyzed with the same multiple-trapping model that is used for the TPC signals [3].

The basic multiple trapping equations are [11]:

$$\frac{\partial n(x,t)}{\partial t} = -\sum_{i}^{m} \frac{\partial n_i(x,t)}{\partial t} - \mu_0 F \frac{\partial n(x,t)}{\partial t} - \frac{n(x,t)}{\tau} + n_0 \delta(t), \tag{1}$$

$$\frac{\partial n_i(x,t)}{\partial t} = \omega_i n(x,t) - \gamma_i n_i(x,t). \tag{2}$$

where x is the distance from one electrode, τ is monomolecular recombination lifetime, $n(x,t)$ is the free carrier density at x and t, $n_i(x,t)$ is the trapped carrier density at the ith localized state at x and t, μ_0 is the microscopic mobility, F is the applied electric field, n_0 is the injected free carrier density, $E_i = i\Delta E$ is the ith energy level below (or above) a mobility edge, $\omega_i = \sigma \nu_{th} g(E_i)\Delta E$ and $\gamma_i = \nu \exp(\frac{E_i}{k_B T})$ are the capture rate constant and release rate at the ith localized state, respectively, σ is the capture cross section, v is the thermal velocity, $g(E_i)$ is the density of state at the ith localized state, ν is the attempt-to escape frequency, K_B is Boltzmann's constant and T is the

measurement temperature. The delta function in Eq. (1) defines the optical excitation for the T-TOF experiment. These equations can be solved using Laplace transforms under the initial and boundary conditions of $n(x,0)=0, n_i(x,0)=0$, and $n(0,t)=0,$

The Laplace transform of Eqs. (1) and (2) using

$$n(x,s)=\int_0^{\infty} n(x;t)\exp(-st)dt \tag{3}$$

The solution of Eqs. (1) and (2) for $n(x,s)$ is

$$n(x,s)=\frac{n_0}{a(s)}\left\{1-\exp\left(\frac{a(s)t_0}{L}x\right)\right\} \tag{4}$$

Where

$$\begin{aligned} a(s) &= s+\sum_i^m \frac{s\omega_i}{s+\gamma_i}+\frac{1}{\tau} \\ &= s+s\int_0^{E_f}\frac{\sigma\nu g(E)}{s+\nu\exp\left(-\frac{E}{k_BT}\right)}dE+\frac{1}{\tau}, \end{aligned} \tag{5}$$

in which s is the Laplace variable and $t_0=\frac{L}{\mu_0 F}$.

Using an approach developed in [6], the following expression can be written:

$$\frac{da(s)}{d\ln s}=s\left[1+\int_0^{E_f}\sigma\nu g(E)h(s,E)dE\right] \tag{6}$$

Where

$$h(E,s)=\frac{\nu e^{-\frac{E}{k_BT}}}{\left(s+\nu e^{-\frac{E}{k_BT}}\right)^2} \tag{7}$$

Making the approximation $h(s,E)\approx\frac{K_BT}{s}\delta(E-E_0)$ where $E_0=K_BT\ln(\frac{\nu}{s})$, we have

$$\frac{da(s)}{d\ln s} = s + \sigma\nu k_B T g(E)$$

For TOF experiment, the photocurrent is given by

$$I(t) = \frac{q\mu_0 F}{L}\int_0^L n(x,t)dx, \qquad (8)$$

which is transformed into

$$I(s) = \frac{q\mu_0 F}{L}\int_0^L n(x,s)dx = \frac{qLn_0}{a(s)^2 t_0^2}\left\{e^{-a(s)t_0} - 1 + a(s)t_0\right\} = \frac{I(0)}{a(s)\ t_0{}^2}\left\{1 - e^{-a(s)t_0} - 1 + a(s)t_0\right\} \qquad (9)$$

where q is the electronic charge and $I(0) = \frac{qn_0\mu_0 F}{L}$.

Computational procedure

To examine the transient photodecay in the case of an exponential distribution of localized states, which has often been found in disordered semiconductors, we have employed the technique of the inverse Laplace transform. The computed transient, were obtained using a numerical algorithm. We calculated the inverse Laplace transform numerically, using the Padé approximation (a rational approximation with polynomials of 8-2degree).

In our case, and in order to construct a current numerically we proceeded with the following steps: as we known, the inverse Laplace of a function is given by

$$I(t) = \frac{1}{2\pi i t}\int_{c'-i\infty}^{c'+i\infty} I\left(\frac{z}{t}\right)e^z dz \qquad (10)$$

according to equation (10), the calculated current can be performed as follows: (i) first, one expresses the expansion of the function in Padé approximation: The Padé approximation of a function is quite similar to a Taylor series, except that the development is a ratio of two polynomials. (ii) secondly, we apply the residual theorem to obtain the desirable function, that is, the calculated current.

Results and discussion

In the case of pure exponential tail, the simulation generates transient decay which has a power-law form as demonstrated in figures 1 and 2.

Fig.1 shows a plot of the simulated transient photocurrents versus time for various characteristic temperatures. It is clearly seen that the transient photocurrent decreases with time. For non-dispersive transport $T_0 = 250K$ the transit time can be obtained at the intersection of the transient photocurrent with the time-axis. Similar results are obtained for dispersive transient photocurrent.

Fig.2 illustrates the current transients at various values of applied electric fields. An interesting point manifested in Fig.2 that the inflection point is not affected by the applied field and thus is not due to transit time but to the monomolecular recombination lifetime. The transit time is much shorter than the monomolecular recombination lifetime. In this case, the inflection points shift toward a shorter time regime by increasing applied electric field. This means that the inflection point is due to the transit time. From these results, we can experimentally distinguish weather or not the inflection point is the charge carrier transit time: if the inflection point becomes shorter with applied electric field, then the inflection point is charge carrier transit time. As a result, the drift mobilities can be determined under the condition that the charge carrier transit time is much shorter than the monomolecular recombination lifetimes.

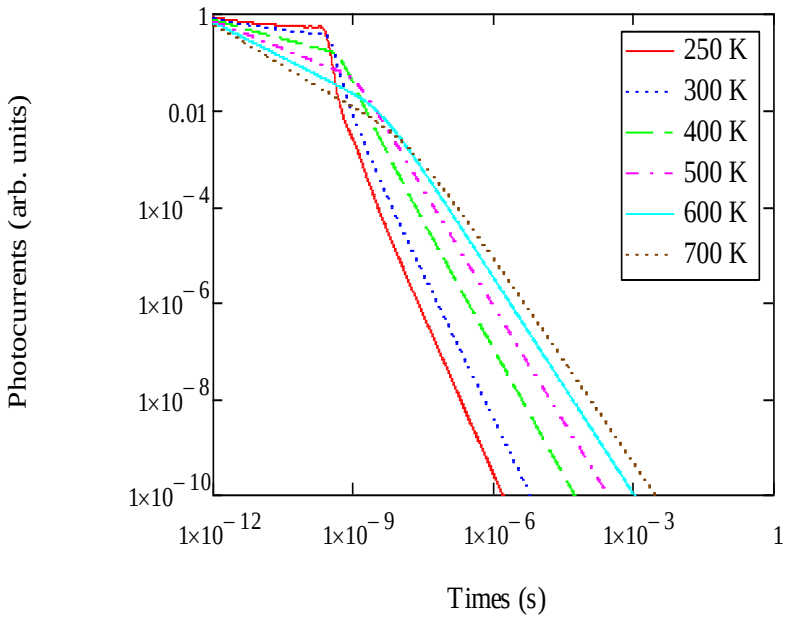

Figure1: Simulated transient photocurrents for different values of T_0

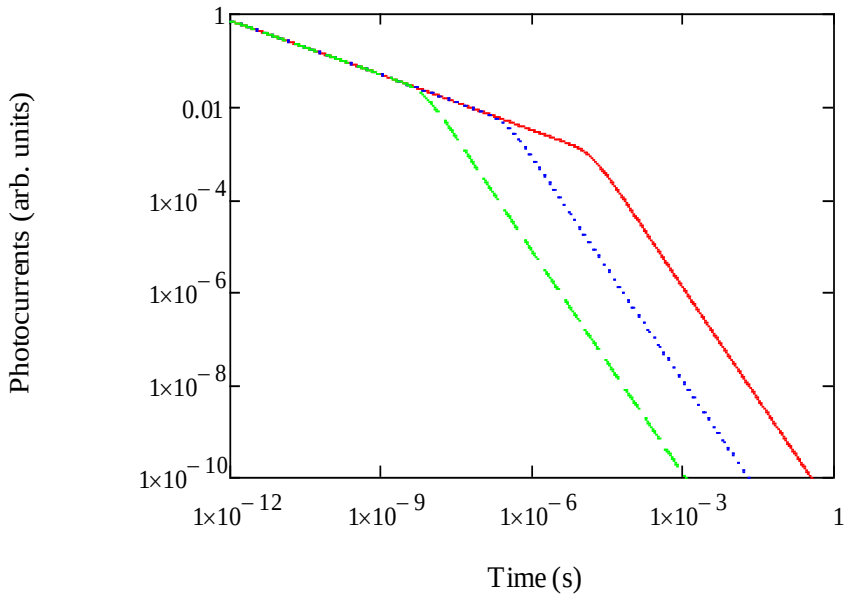

Figure2: Simulated transient photocurrents for different values of applied electric field:

$$\left(4\times10^{3},4\times10^{4}\text{and}4\times10^{5}\right)\frac{\text{V}}{\text{cm}}$$

Conclusion

We have demonstrated that the transient photodecay technique is capable to detecting the presence of energy distribution localized states and our studies provide a means of assessing to any structure in the trap distribution. In order to check the validity of these methods, the photocurrents obtained with inverse Laplace transform technique from simulation were compared to the measured transient photocurrents for any trap level model. The numerical results confirm the image of the density of localized states.

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