Deep Trap Modelling and Transient Measurements of a-Si:H p-i-n Diodes

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Abstract

The behaviour of a-Si:H p-i-n diodes is simulated using a straight-forward model based on rate equations for deep trapping. The absolute levels of simulated currents agree well with measured results on state-of-the-art a-Si:H p-i-n diodes. Characteristic features observed in measurements are also seen in the simulated results. The model is based on Euler’s method of numerically solving the transport equations. The traps are modelled as two Gaussian shaped functions near the middle of the band gap.

1. Introduction

For a-Si:H it is predicted that the transient time constants can have a very wide range, which can cause problems in device operation. An example is image lag in sensor systems. With a continuous distribution of traps in a band gap of ~1.85 eV the distribution of emission constants arising from deep trapping effects can be in the time range 10^{-3} to 10^{5} s. This is previously known and also shown by reverse-bias current measurements performed by ref [1].

The purpose of this work is to make a straight-forward model of an a-Si:H p-i-n diode that takes physical characteristics into account. The model is to be used in circuit-simulations to be able to design circuitry that compensates for unwanted effects.

Most of the previous models of transient behaviour of a-Si:H p-i-n devices are very detailed and have mainly studied the trapping effects of tail states with characteristic features observed in the time region 10^{-13} - 10^{-3} s [2,3]. There are also examples of advanced models taking both deep and tail states into account [4]. Since the most important time region for our system application is from a few microseconds to ~60 ms, we are mainly interested in the time region above 1 µs and up to 10 s, and the effects of deep trapping seen as a system behaviour in this region.

In this work, the model is based on standard transport equations, solved numerically by Euler’s method. Only contribution from deep states is considered.

2. Trap equations

The transitions included in the model are

- capture of an electron or a hole to an empty electron or hole trap,
- emission of an electron or a hole from an occupied trap and
- recombination by the capture of an electron/hole to a trap occupied by a hole/electron.

In this first model the geometric dependency of the field is excluded. We assume that the traps dominate the behavior of the diode in the modeled time scale. All variables are therefore considered as an average over the x-axis.

In the model, 50 discrete energy levels, E_i, are used. This means that the number of traps, N_t, and P_t, and the emission constants, e_n,i and e_p,i, are vectors. The model calculates the time dimension for the trapped carrier density, n(t), and the rate of carrier trapping, \frac{\partial n}{\partial t}, for the entire energy region simultaneously, and creates two dimensional matrices in energy and time. In the last equation when the free carrier density n(t) is calculated, \frac{\partial n}{\partial t} is summarized over all energy levels. The carrier loss at the contacts is accounted for by the last term in n(t) and p(t), respectively.

\frac{\partial n_i(t)}{\partial t} = w \cdot v_e \cdot \sigma_e \cdot n(t-1) \cdot (N_e - n_i(t-1)) - w \cdot e_n \cdot n_i(t-1)

\frac{\partial p_i(t)}{\partial t} = w \cdot v_h \cdot \sigma_h \cdot p(t-1) \cdot (P_p - p_i(t-1)) - w \cdot e_p \cdot p_i(t-1)
The light pulse is modelled by the generation of electron-hole pairs, \( G_n(t) \). The generation of electron-hole pairs is assumed to be uniform throughout the volume, since the incident light is considered to be of long wavelength (red) and the devices are thin. The current, \( i(t) \), is finally calculated as

\[
n(t) = n(t-1) + \frac{\partial n(t-1)}{\partial t} \cdot dt - w \cdot v_e \cdot \sigma_{pm} \cdot n(t-1) \cdot p(t-1) \cdot dt
\]

\[
p(t) = p(t-1) + \frac{\partial p(t-1)}{\partial t} \cdot dt - w \cdot v_p \cdot \sigma_{np} \cdot n(t-1) \cdot p(t-1) \cdot dt
\]

\[
N = n(t) + G_n(t-1) - \sum_{E \in \{E_n, E_p\}} \frac{\partial n(t-1)}{\partial t} \cdot dt - w \cdot v_e \cdot \sigma_{pm} \cdot \sum_{E \in \{E_n, E_p\}} n(t-1) \cdot p(t-1) \cdot dt - n(t-1) \cdot E / \mu_n \cdot dt
\]

\[
p(t) = p(t-1) + G_p(t-1) - \sum_{E \in \{E_n, E_p\}} \frac{\partial p(t-1)}{\partial t} \cdot dt - w \cdot v_p \cdot \sigma_{np} \cdot \sum_{E \in \{E_n, E_p\}} p(t-1) \cdot n(t-1) \cdot dt - p(t-1) \cdot E / \mu_p \cdot dt
\]

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\[
i(t) = A \cdot q \cdot E \cdot \left( n(t) \cdot \mu_n + p(t) \cdot \mu_p \right)
\]

The emission constants \( e_{nt}, e_{nt} \) are modelled based on detailed balance at equilibrium, when the number of captured electrons is equal to the emitted electrons.

\[
e_{nt} = v_e \cdot \sigma_n \cdot N_e \cdot e^{(E_t - E_c)/kT}
\]

The distribution function for the deep traps is assumed to be two Gaussian shaped functions near the middle of the bandgap, as shown in Fig. 1. The electron and hole traps are considered separately. The constant, \( a \), is chosen so that the total number of traps is close to \( 10^{21} \text{ m}^{-3} \), which corresponds to estimated results from steady-state generation current in [1].

The constants \( E_n \) and \( E_p \) place the center of the trap peaks at 6.65 and 6.45 eV respectively. This is 0.8-1 eV below the conduction band edge, and a similar distribution of deep traps was used by [4]. The distribution of deep traps also corresponds well to measurements done by [5].

### Table 1. Constants

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal velocity ( v_e )</td>
<td>10^5 m/s</td>
</tr>
<tr>
<td>Electron mobility ( \mu_n )</td>
<td>10^-4 m^2/Vs</td>
</tr>
<tr>
<td>Hole mobility ( \mu_p )</td>
<td>3·10^-7 m^2/Vs</td>
</tr>
<tr>
<td>Density of states at the conduction band ( N_c )</td>
<td>2·10^27 m^-3</td>
</tr>
<tr>
<td>Density of states at the valence band ( N_v )</td>
<td>2·10^27 m^-3</td>
</tr>
<tr>
<td>Capture cross-section, electrons to traps ( \sigma_n )</td>
<td>2.7·10^-19 m^2</td>
</tr>
<tr>
<td>Capture cross-section, electron to occupied hole traps ( \sigma_{np} )</td>
<td>1.3·10^-14 m^2</td>
</tr>
<tr>
<td>Capture cross-section, holes to traps ( \sigma_p )</td>
<td>8·10^-19 m^2</td>
</tr>
<tr>
<td>Capture cross-section, holes to occupied electron traps ( \sigma_{pn} )</td>
<td>2·10^-15 m^2</td>
</tr>
</tbody>
</table>

The parameters used in the simulations are given in Table 1. Most of the parameters are found in reference [6], in which the cross-sections are calculated from measured results and measured values of density of states at conduction and valence band edges are presented. (Other parameters in the trap equations include the electric field, \( E \), the area of the diode, \( A \), the thickness of the i-layer, \( w \), the elementary charge, \( q \), the conduction and valence band edge energies, \( E_c \) and \( E_v \).)

### 3. Experimental

The measurements have been performed on state-of-the-art PECVD- diodes. The dimensions are 120 micron square with an i-layer thickness of 900 nm \( (w) \). The bias voltage was held constant during current measurements. We used a current preamplifier, (Stanford Research Systems SR 570), and sampled the output by an I/O card (PCI-DAS4020/12). The bias voltage used was -1V, -2V or –5V. The illumination source is a manually shuttered DC source (Optronics Laboratories OL 462).
In this first attempt to model the measured behaviour, long illumination pulses are considered. The diodes were therefore exposed to a light step from dark to light or from light to dark. In the present measurements, the built-in noise-filter in the current preamplifier, was used and set to 30 Hz.

4. Results

When a current generated from a light pulse is simulated, the absolute levels of the current are around 1 nA in dark and around 10 nA in light, as seen in Fig. 3. These simulated current levels are well in agreement with the current levels that were measured and are shown in Fig. 4 and 6. The modelled incident light intensity and electron-hole pair generation, \( G_n \), in Fig. 3 and 5 was \( 5 \times 10^{18} \text{ m}^{-2}\text{s}^{-1} \) and \( 1 \times 10^{20} \text{ m}^{-2}\text{s}^{-1} \), respectively. In the measurements shown in Fig. 4, the incident intensity was 8 W/m², which can be approximated to a photon flux of \( 5 \times 10^{19} \text{ m}^{-2}\text{s}^{-1} \), by calculation of the energy of incident photons with 600 nm wavelength and an average quantum efficiency of 60% (from [7]).

Some of the physical characteristics observed in the measurements can also be observed in the simulated results. Fig. 4 shows measured curves from the exposure of a light step from dark to light. The curve measured with -5 V bias shows a small linear part before the current reach a more steady-state like behaviour. This linear region can also be shown in simulated results see Fig. 5. The time scale for this linear region is the same for both simulations and measurements. The linear part in the modelled curve depends on the slower increase of the hole current.

The measurement on photocurrent decay is shown in Fig. 6. Due to filtering effects and manual shuttering the time it takes for the current to decrease appears to be long. In the upper curve a more slowly decreasing lag-current can be seen.

The simulated photo current decay is shown in Fig. 7, where the decreasing current shows a similar behaviour as in the measured results. In Fig. 8 it is shown that the current tail depends on the large number of free holes moving slowly through the material.
5. Discussion

Using a simple straight-forward model excluding space-charge effects it is possible to simulate the behavior of a reverse-biased p-i-n diode and make a physical explanation. The absolute current levels correspond to measured results. The bias dependence, however, is not entirely correct. The linear increase of the current with higher bias shown in Fig. 3 differs from the measured bias dependence shown in Fig. 4. We have in other measurements found a Poole-Frenkel-like behavior, as also noted by [1], that can be the cause of this discrepancy and we intend to include this effect in an improved model. Also the dark current level might be further improved. In this first attempt we have modeled the dark current as a small illumination corresponding to our measurements. This is motivated by the fact that our “dark” levels are not measured in complete darkness. The linear region found in the photo current increase as the illumination is on can be explained in the simulations by the slow response of the hole current. The densities of trapped and free holes in the i-layer of the diode are at very high level, compared to the electrons, during the entire illumination pulse. The free electrons are at a much lower level since their mobility is higher and they can escape faster through the contacts. The decay of the current after removal of the illumination is shown to depend on a high density of free and trapped carriers stored in the material mainly due to low mobility. The free holes are retrapped before they reach the contacts. A difference in shape of the curves in Fig. 3 and 5 is also observable. The higher intensity of photon flux in the simulation in Fig. 5, results in a faster generation of holes than the escape rate. In this simulation the holes then contribute to the current level when the density reaches a threshold value.

6. Conclusion

We have shown a simple model of a-Si:H p-i-n diodes based on transport equations, including deep trapping effects. This first model show some of the characteristic physical features of a-Si:H diodes visible in measurements.

7. Acknowledgements

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8. References