Theoretical model for spatial separation of dominating recombination region in a-Si:H/c-Si structures

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Abstract. In this paper we describe a theoretical model for spatial quantitative separation and determination of dominating recombination region in structures with amorphous/crystalline silicon heterojunction. This model is based on analysis of ideality factor, experimentally obtained from open circuit voltage dependence of generation rate; characteristic energy, corresponding to the maximum possible quasi Fermi level separation, experimentally obtained from temperature dependence of open circuit voltage. Compared to the existing approaches in this work we consider recombination in the bulk of amorphous silicon.

1. Introduction
There is a model [1] for mathematical separation of total recombination rate \( R_{\text{total}} = \sum R_i \), described by SRH statistics. The obtained values correspond to the different spatial regions of photoactive layers in solar cells. Grover [1] spatially separated investigated structure of CIGS and a-Si/c-Si solar cells and marked 3 regions: interface, depletion region and quasi neutral part of the base (Figure 1). This approach allows to define dominating recombination region and calculate contribution of every region on total recombination rate. In this case discontinuity equation under open circuit conditions:

\[
G = R_i + R_b + R_d.
\]

(1)

where \( G \) — generation rate, \( R_i \) — recombination rate at the interface \( R_i = R_i^0 \beta^2 \), \( R_b \) — recombination rate in the quasi-neutral part of the base \( R_b = R_b^0 \beta^2 \), and \( R_d \) — recombination rate in the depletion region \( R_d = R_d^0 \beta \).

Grover denoted each recombination rate as a multiplication of light dependent \( \beta \) and light independent values \( R_i^0, R_b^0, R_d^0 \).

\[
G_{\text{avg}} = [R_i^0 + R_b^0] \beta^2 + R_d^0 \beta.
\]

(2)

Here \( \beta \) is defined from the difference of quasi Fermi levels that equals open circuit voltage \( V_{oc} \):

\[
V_{oc} = \frac{kT}{q} \ln \frac{n_e p_h}{n_i^2} = \frac{kT}{q} \ln \beta^2.
\]

(3)

with \( n_e \) and \( p_h \) — total concentration of electrons and holes respectively, \( n_i \) — intrinsic charge carrier concentration, \( k \) — Boltzmann constant, \( T \) — temperature, \( q \) — elementary charge.

This approach suggests to define diode ideality factor \( n \) from experimental \( G(V_{oc}) \) measurements and links \( n \) with \( \beta \) and \( R_i^0, R_b^0, R_d^0 \).
Solving quadratic equation (2) about $\beta$ and considering (3) and (4):

$$n(G) = \frac{k_2 G}{\sqrt{1+k_2 G}[\sqrt{1+k_2 G}-1]}$$

with

$$k_1 = \frac{R_1^0 + R_0^d}{2*(R_0^d + R_0^b)^2}, \quad k_2 = \frac{4+2*(R_1^0 + R_0^d)}{(R_0^d + R_0^b)^2}$$

Considering the fact that ideality factor provides information about dominating recombination region discontinuity equation could be simplified:

$$G = (R_1^0 + R_0^d)\beta^2, \quad \text{or} \quad G = R_0^d\beta$$

However, despite the fact that this model developed for heterojunction amorphous/crystalline silicon structures, recombination in the bulk of amorphous silicon is not considered there. Moreover recombination in a-Si could be described on the basis of classical SRH approach and amphoteric defect model [2]. It should be considered for describing recombination in amorphous silicon.

In this paper we extended Grover’s model and analytically considered recombination in the bulk of amorphous silicon layer.

2. Model
We spatially separate a-Si/c-Si structure and mark four recombination regions: interface $R_1$, depletion region $R_d$, quasi neutral part of the base $R_b$ and the bulk of amorphous silicon $R_a$ (Figure 1).

![Figure 1](image-url)

Figure 1 – Spatial separation of recombination regions in a-Si:H/c-Si cells by the Grover model (left) and proposed model (right)

According to [1] we denote recombination rate in each region as a multiplication of light dependent and light independent values. We denote recombination rate in amorphous silicon $R_a$ similarly, that provides the extended equation of generation-recombination balance (8):

$$G = R_1 + R_b + R_d + R_a$$

Following Steingrube [2] and Olibet [3] recombination rate in the bulk of amorphous silicon could be defined considering classical SRH statistics and amphoteric defect model:
These equations consider concentration of traps $N_t$ or dangling bonds $N_{DB}$, thermal velocity $v_{th}$, concentration of free electrons $n_f$ or holes $p_f$, capture cross section of holes $\sigma_p$ and electrons $\sigma_n$ with positive $\sigma_p^+$, neutral $\sigma_n^0$, and negative $\sigma_p^-$ charge for amphoteric states. However in the case of n-type, for instance, these equations could be simplified [3]:

$$R_{DB} = \frac{n_f\sigma_n^0 + p_f\sigma_p^0}{p_f\sigma_p^0} v_{th} N_{DB}.$$  \(10\)

In this case there is no functional difference between SRH and amphoteric defect model. Considering that recombination in amorphous silicon corresponds to the case of non-ideal diode $n \geq 2$ [4], we denote $R_a = R_0^a \beta$.

Replacing recombination rate by multiplication:

$$G = (R_l^0 + R_b^0)\beta^2 + (R_d^0 + R_a^0)\beta,$$  \(12\)

where $R_l^0$, $R_b^0$, $R_d^0$, $R_a^0$ light independent values.

The proposed model is based on analysis of ideality factor, experimentally obtained from open circuit voltage dependence of generation rate (Figure 2). The obtained value allows to estimate dominating recombination in the quasi neutral base or at the interface ($n \sim 1$); and in the depletion region or in the bulk of amorphous silicon ($n \sim 2$). In the case of $n \gg 2$, we assume that charge carrier recombine predominantly in a-Si [4]. Therefore, defined ideality factor provides simplified equation of generation-recombination balance (13), considering only dominating regions.

$$G = (R_l^0 + R_b^0)\beta^2,$$  \(13\)

To calculate the prevailing value in the sums $R_l^0 + R_b^0$ and $R_d^0 + R_a^0$, we, considering Grover [1], suggest to measure temperature dependence of open circuit voltage (Figure 2).

Figure 2 – Dependence of open circuit voltage from generation rate and temperature dependence of open circuit voltage with extrapolation of the obtained data to estimate maximum possible quasi Fermi level separation [1]
Extrapolation of this dependence allows to define a characteristic energy, corresponding to the maximum possible quasi Fermi level separation, which equals:

1. \(E_a = E_g(c - Si)\) c-Si band gap, in the case of dominating recombination in quasi neutral part of crystalline silicon or 
\(E_a = \varphi_{b,o}(c - Si)\) interface potential, in the case of dominating recombination at the interface, \(n\sim 1\);

2. \(E_a = E_g(a - Si; H)\) a-Si mobility gap, in the case of dominating recombination in the bulk of amorphous silicon or 
\(E_a = E_g(c - Si)\) c-Si band gap, in the case of dominating recombination in the depletion region, \(n\sim 2\).

3. Conclusion
The proposed model allows to separate quantitatively recombination regions and to calculate maximum value of recombination rate in the corresponding region, which significantly determines total recombination rate in heterojunction structures based on a-Si/c-Si. The described theory, extended by experimental measurements, provides these tasks. It this case the approach consists of the following steps:

- experimental determination of ideality factor from \(G(V_{oc})\) dependence;
- analysis of pair of dominating regions according to ideality factor equals 1 or 2 (\(\geq 2\));
- measuring temperature dependence of open circuit voltage and extrapolation of the obtained data to define characteristic energy;
- considering value of the characteristic energy estimation of dominating region quantitatively.

Despite that other recombination rates except the dominating value are neglected and solution is based on the simplified discontinuity equation, the physical and mathematical aspects of the model could be extended for the case of total generation-recombination balance \(G = (R_0^b + R_0^a)\beta^2 + (R_d^0 + R_a^0)\beta\), that will provide all of the recombination rate values.

References
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