

# Modelling the light induced metastable effects in amorphous silicon

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We present results of computer simulations of the light induced degradation of amorphous silicon solar cells. It is now well established that when amorphous silicon is illuminated the density of dangling bond states increases. Dangling bond states produce amphoteric electronic mid-gap states which act as efficient charge trapping and recombination centres. The increase in dangling bond states causes a decrease in the performance of amorphous silicon solar cells. To show this effect, a modelling approach has been developed which uses the density of localised states with exponentially increasing band-tails and dangling bond defect states distribution chosen according to the defect pool model. The calculation of the evolution of dangling bond state density during illumination has been achieved through a dynamic scaling relation derived from a defect creation model. The approach considers the amphoteric nature of the dangling bond state and thus accounts for the contributions of the different charge states of the dangling bond during the degradation process. This paper attempts to describe the simulation approach which calculates the defect density as a function of energy, position in the solar cell and illumination time. In excellent agreement with other workers, our simulation results show that the increase in the density of neutral dangling bond states during illumination is higher than of the charged states.

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**1 Introduction** Since the discovery of light induced metastable defects, the Staebler-Wronski effect (SWE) [1] in hydrogenated amorphous silicon (a-Si:H), the study of metastability in this material has been an active field of research [2]. Several experiments and a variety of theoretical models have been employed to explain this phenomenon. However, owing to the complex nature of the electronic properties of hydrogenated amorphous silicon, the underlying physics of metastability in this material is still not fully explained or understood. The subsequent studies carried out to address this problem have yielded important results which form a viable base for continued research progress. It is now known from direct experimental evidence [3] that the light induced degradation of hydrogenated amorphous silicon is a result of the creation of metastable midgap defect states, the dangling bonds (DBs). The dangling bond defect may have three charge states; positive when empty ( $D^+$ ), neutral when singly occupied ( $D^0$ ) or negative when occupied by two electrons ( $D^-$ ). In the neutral state, the

dangling bond can trap either electrons or holes. To study metastability in amorphous silicon, a thorough investigation of the contributions of the various charge states of the dangling bond to the degradation mechanism is therefore required.

Based on distinct experimental scenarios, several microscopic processes have been proposed to explain the SWE. Theoretical advances such as the defect pool model (DPM) [4] have provided the concepts necessary to describe the density and distribution of DB states at thermal equilibrium. The defect pool model assumes that the cost of forming a defect at any particular site in amorphous silicon depends on its charge state and the position of the Fermi level. The concept of the defect pool model is widely accepted, but unfortunately it cannot describe the DB states distribution during illumination of amorphous silicon, an entirely non-equilibrium process. Of the many microscopic models which have been put forward to explain the defect creation mechanism in amorphous silicon,

the Stutzmann et al. (SJT) [5] model is widely quoted and accepted. According to the SJT model, light induced degradation in the electronic properties of a-Si:H is a result of a weak bond-dangling bond conversion mechanism arising from the direct tail-to-tail recombination (bimolecular) process. The DPM was developed from the weak-bond-dangling-bond conversion model to account for the increase in the defect concentration upon doping [6] or upon light soaking. The DPM assumes that  $D^0$ ,  $D^-$  and  $D^+$  levels are associated with different types of dangling bonds, created in different energy ranges of the defect pool.

The study of metastability in amorphous silicon is therefore complex and it requires a dynamic approach which describes the density and nature of the dangling bond states, their redistribution and evolution during illumination. Computational simulations have been applied to study the defect evolution during illumination of a-Si:H solar cells. Most of these studies have used a simplified approach of simulating the annealed and degraded state by varying the overall density of the dangling bonds [7]. This approach does not incorporate the roles different charge states of the DB play in the light induced degradation mechanism. The purpose of this work is to investigate the degradation kinetics of a-Si:H solar cells in a manner that provides information on changes in both external and microscopic parameters of the solar cell as a function of illumination time. Utilizing the Stutzmann et al. [5] defect creation model, a dynamic scaling relation for the evolution of gap states during illumination of a-Si:H has been developed. The scaling relation is a quasi-static (non-equilibrium) formulation, which has been applied to vary the three Gaussians of the dangling bond state as described by the defect pool model. In accordance with the SJT model, the non-radiative tail-tail recombination is the driving force for the creation of the dangling bonds. Using the non-radiative recombination of spatially correlated band tail states for defect creation, an iterative scheme was incorporated in the device simulator program ASA (Amorphous Semiconductor Analysis program developed at the Technical University of Delft) to track the defect density as a function of energy, illumination time and position in the solar cell. A pre-factor in the scaling formula which is physically related to the efficiency of SWE and the different capture rate coefficients of all charge states of the dangling bond was used as the fitting parameter.

**2 Kinetics of defect creation** The SJT model [5] relates the density of dangling bond states to the intensity and duration of light exposure. In the context of this model, electrons trapped in the antibonding orbital (conduction band tail) and holes trapped in the bonding orbital (valence band tail) form excitons. Recombination of these band tail excitons release energy (approximately 1.5 eV) which is sufficient to break a weak Si-Si bond and lead to the creation of new midgap defects. The DBs generated through the recombination driven kinetics control the density of charge carriers. The model gives the following rate equation

for the increase of the defect density ( $N_r$ ) during illumination:

$$dN_r / dt = C_{sw} C_t n p \quad (1)$$

where  $C_t$  is the coefficient for the tail-tail transitions,  $C_{sw}$  is the coefficient for the creation of new dangling bonds which is widely known as the Staebler-Wronski coefficient,  $n$  and  $p$  are carrier concentrations. The carrier concentrations  $n$  and  $p$  are given by:

$$n = G / C_n N_r \quad \text{and} \quad p = G / C_p N_r \quad (2)$$

where  $G$  is the carrier generating rate in  $\text{m}^{-3}\text{s}^{-1}$ ,  $C_n$  and  $C_p$  are the capture rate constants for electrons and holes into dangling bond states. Substituting Eq. (2) into Eq. (1) yields the following expression

$$dN_r / dt = \frac{C_{sw} C_t G}{C_n C_p N_r^2} \quad (3)$$

Equation (3) can be integrated to give

$$N_r^3(t) - N_r^3(t_0) = 3C_{sw} \frac{C_t G^2 t}{C_n C_p} \quad (4)$$

where  $N_r(t_0)$  is the as-deposited defect density and  $N_r(t)$  is defect density after time  $t$  of illumination.

Equation (4) can be simplified to yield the number of dangling bonds as a function of illumination time  $t$ .

$$N_r(t) = N_r(t_0) + [3C_{sw} C_t / C_n C_p]^{1/3} G^{2/3} t^{1/3} \quad (5)$$

Equation (5) gives the widely experimentally observed nonlinear time-dependence of the light generated defect density namely  $N_r \propto t^{1/3}$

**3 Formulation of the scaling relationship for the defect increase** A major consideration in this study is to show how the increase in dangling bond density of states during illumination affects the output of a solar cell. A dynamic scaling formula which can scale a given defect density distribution is derived from the SJT defect creation formulation. This is obtained by dividing both sides of Eq. (5) by  $N_r(t_0)$  which is the as-deposited defect density.

$$\frac{N_r(t)}{N_r(t_0)} = 1 + \left[ \frac{3C_{sw} C_t}{C_n C_p} \right]^{1/3} G^{2/3} t^{1/3} \frac{1}{N_r(t_0)} \quad (6)$$

We now introduce a prefactor

$$C_{LS} = \frac{[3C_{sw} C_t / C_n C_p]^{1/3}}{N_r(t_0)} \quad (7)$$

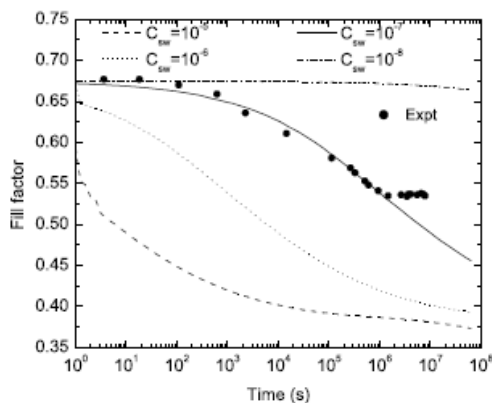
Substituting Eq. (7) into Eq. (6) and letting the ratio  $N_r(t)/N_r(t_0) = k(t)$  leads to a dimensionless scaling factor

$$k(t) = 1 + C_{LS} R^{2/3} t^{1/3} \quad (8)$$

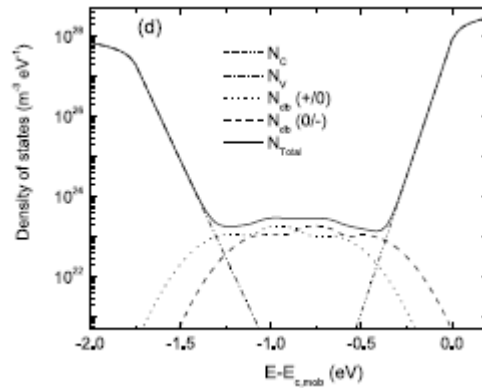
In Eq. (8) the generation rate  $G$  is replaced with the dangling bond mediated recombination rate  $R$  in  $\text{m}^{-3}\text{s}^{-1}$ .

The scaling factor  $k(t)$ , determines the increase in the defect density at a given time  $t$  (in seconds). At  $t=0$ ,  $k=1$  implying that the number of recombination centres is equal to the as-deposited defect density  $N_r(t_0)$  and the change in this number is determined by changes in the last term of Eq. (8). Assuming that the capture rate coefficients  $C_p$ ,  $C_n$ , and  $C_i$  remain constant during illumination, then the variation in the prefactor  $C_{LS}$  is dependent on the values of  $C_{SW}$ , which is the coefficient for the creation rate of new dangling bonds.

**4 Computational procedure** To describe the defect creation process in a-Si:H requires different creation rates for the different charge states of the dangling bond. This can be illustrated by assigning different values of  $C_{SW}$  for different charge states of the DB during light soaking. Based on Eq. (8) we introduced the scaling factors  $k_e$ ,  $k_h$  and  $k_z$  with different values of  $C_{SW}$  to simulate the degraded state of a cell. These factors correspond to dangling bond states  $D^+$ ,  $D^-$  and  $D^0$  respectively. The predictions of various calculations based on the defect pool model show that the ratio of charged-to-neutral defects at equilibrium (in the as deposited state) is between three and seven [8], by light soaking the solar cell, this ratio drops to one. Based on this prediction, the scaling factors for individual charge states of the dangling bond were varied using the parameter  $C_{SW}$  to fit the experimental data. The implicit iterative structure for increasing the DB density of states (DOS) in a solar cell began with the calculation of the as deposited DOS according to the defect pool model  $N_{db}(E, x, t_0)$ .



**Figure 1** The fill factor as function of illumination time for different  $C_{SW}$ .



**Figure 2** The DOS distribution calculated for the centre of the cell and used to fit the degraded state.

**5 Results and discussion** The simulated and experimental fill factor of a solar cell as a function of illumination time is shown in Fig. 1. The simulations were achieved with different values of  $C_{SW}$ . It is observed that the experimental curve is approximately fitted when  $C_{SW} = 1.0 \times 10^{-7}$ . This implies that for every  $1.0 \times 10^7$  recombinations only one such recombination leads to the creation of a new dangling bond. It is also noticed that the time at which saturation is achieved is different for experimental and simulated curves. This observation means that modeling the light induced degraded state of a-Si:H solar cells require the knowledge of both the defect creation and annealing rates. Changes in the DOS distribution as function of energy and position in the solar cell for different stages of light soaking were obtained. Shown in Fig. 2 is the typical DOS distribution calculated for the centre of the solar cell and used to fit the degraded state of the cell. In agreement with other workers, the results show that the increase in the density of neutral dangling bond states during illumination is higher than of the charged states. Thus with this approach it is possible to study the contributions of the different charge states of the DB during the photo induced degradation of a-Si:H solar cells. In summary, this paper describes an approach which calculates the defect density of states in a-Si:H solar cell as a function of energy, position and illumination time.

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