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Citation: *Journal of Applied Physics* **105**, 044502 (2009);

View online: <https://doi.org/10.1063/1.3078044>

View Table of Contents: <http://aip.scitation.org/toc/jap/105/4>

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Determination of the mobility gap of intrinsic $\mu\text{c-Si:H}$ in $p-i-n$ solar cells

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(Received 11 August 2008; accepted 30 December 2008; published online 17 February 2009)

Microcrystalline silicon ($\mu\text{c-Si:H}$) is a promising material for application in multijunction thin-film solar cells. A detailed analysis of the optoelectronic properties is impeded by its complex microstructural properties. In this work we will focus on determining the mobility gap of $\mu\text{c-Si:H}$ material. Commonly a value of 1.1 eV is found, similar to the bandgap of crystalline silicon. However, in other studies mobility gap values have been reported to be in the range of 1.48–1.59 eV, depending on crystalline volume fraction. Indeed, for the accurate modeling of $\mu\text{c-Si:H}$ solar cells, it is paramount that key parameters such as the mobility gap are accurately determined. A method is presented to determine the mobility gap of the intrinsic layer in a $p-i-n$ device from the voltage-dependent dark current activation energy. We thus determined a value of 1.19 eV for the mobility gap of the intrinsic layer of an $\mu\text{c-Si:H}$ $p-i-n$ device. We analyze the obtained results in detail through numerical simulations of the $\mu\text{c-Si:H}$ $p-i-n$ device. The applicability of the method for other than the investigated devices is discussed with the aid of numerical simulations. © 2009 American Institute of Physics. [DOI: 10.1063/1.3078044]

I. INTRODUCTION

Hydrogenated microcrystalline silicon ($\mu\text{c-Si:H}$) is an attractive material for thin-film silicon solar cells. In comparison to hydrogenated amorphous silicon ($a\text{-Si:H}$), $\mu\text{c-Si:H}$ is more stable to light exposure and has a lower bandgap. In particular the “micromorph” concept consisting of an $a\text{-Si:H}$ top cell and a $\mu\text{c-Si:H}$ bottom cell¹ is a promising candidate for cheap and relatively stable thin-film silicon solar cells. With this type of solar cells Yamamoto *et al.* demonstrated a solar cell with an initial efficiency of 14.1%.²

Modeling of $\mu\text{c-Si:H}$ silicon is complicated by its complex microstructural properties involving a mixed phase of crystalline and amorphous tissues, grain boundaries, inhomogeneity in the growth direction, and columnar structure. The complex structural properties give rise to complex properties of electronic transport in the material, impeding a detailed analysis of its optoelectronic properties. In particular, the value of the mobility gap is controversial. Often a value similar to the bandgap of $c\text{-Si}$ (1.1 eV) is used.³ In some other studies, however, mobility gap values have been reported in the range of 1.48–1.59 eV,^{4,5} depending on crystalline volume fraction. For modeling of $\mu\text{c-Si:H}$ materials, it is essential that the mobility gap is accurately determined.

This paper introduces a method to determine the mobility gap of $\mu\text{c-Si:H}$ using the dark current activation energy of $\mu\text{c-Si:H}$ $p-i-n$ devices. We derive a simple analytical model that describes the dark current activation energy and used it to extract the mobility gap of the intrinsic layer of experimental $p-i-n$ devices. As our analytical model is based on several approximations we compare the analytical model with detailed numerical simulations.

The here presented method is, in principal, not limited to $\mu\text{c-Si:H}$ $p-i-n$ devices. Primary assumptions are that the recombination in the dark can be approximated with Shockley–Read–Hall (SRH) recombination, originating from midgap states in the intrinsic layer. To investigate the applicability of the analytical model on other than the investigated devices, we used detailed numerical simulations to study the influence on the dark current activation energy of the band tails, of an amorphous incubation layer, and of a defect-rich interface layer.

II. DETERMINATION OF THE MOBILITY GAP IN $\mu\text{c-Si:H}$ SOLAR CELLS

The dark current is written as the integral of the recombination through the device including surface recombination at the contacts. Recombination in $a\text{-Si:H}$ and $\mu\text{c-Si:H}$ materials is dominated by recombination via dangling bond and tail states. These recombination processes are limited by the minority carrier concentration. As in the doped layers and at the contacts the minority carrier concentrations are low, the recombination in $a\text{-Si:H}$ and $\mu\text{c-Si:H}$ $p-i-n$ devices is dominated by recombination in the intrinsic layer. We therefore approximate the dark current through this type of $p-i-n$ device by the integral of the recombination rate in the intrinsic layer,

$$J = q \int_0^W R(x) dx, \quad (1)$$

where W is the width of the intrinsic layer, q is the elementary charge, and $R(x)$ is the recombination as a function of the position x . In the next two sections we will derive an expression for the thermal activation energy of Eq. (1). In our derivation we approximate the recombination via the amphoteric dangling-bond states with SRH recombination (i.e.,

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the decoupled approach). The derivation presented here is similar to the derivation of the dark J - V characteristics of a -Si:H p - i - n devices from van Berkel *et al.*⁶ However, in order to understand under which circumstances the determined expressions for the dark current activation energy are valid, it is useful to explicitly derive the activation energy of SRH recombination processes as a function of position and trap energy in a p - i - n device. We therefore first derive general expressions for the thermal activation energy of SRH recombination as a function of trap energy in Sec. II A. In Sec. II B we will apply the results of Sec. II A to a p - i - n device and determine the dark current activation energy.

A. Activation energy of SRH recombination

In the following derivation we take abrupt mobility edges. Furthermore, we assume that the capture cross sections for electrons and holes are equal ($\sigma_n = \sigma_p = \sigma$) and we consider equal values for the effective density of states in the valence and conduction bands ($N_c = N_v = N$). Thus the electron concentration n and the hole concentration p are described by

$$n = N \exp\left(\frac{E_{fn} - E_c}{kT}\right), \quad (2)$$

$$p = N \exp\left(\frac{E_v - E_{fp}}{kT}\right), \quad (3)$$

where E_{fn} and E_{fp} are the quasi-Fermi levels for electrons and holes, respectively, and E_c and E_v are the conduction-band and the valence-band mobility edge, respectively.

The recombination efficiency η_R is defined as the recombination per energy state at energy E_t . Thus we write the total recombination rate as

$$R = \int_{E_v}^{E_c} N_t(E_t) \eta_R(E_t) dE_t, \quad (4)$$

where N_t is the number of trap states at energy E_t . By applying the Taylor and Simmons approximation⁷ for the recombination efficiency of a trap and taking the above listed approximations into account, we write for the recombination efficiency of a trap,

$$\eta_R(E_t) = \begin{cases} v_{th} \sigma \frac{np}{n+p} \left[1 + \exp\left(\frac{E_t - E_{fn_t}}{kT}\right) \right]^{-1}, & E_t > E_{\mu}/2 \\ v_{th} \sigma \frac{np}{n+p} \left[1 + \exp\left(\frac{E_{fp_t} - E_t}{kT}\right) \right]^{-1}, & E_t < E_{\mu}/2, \end{cases} \quad (5)$$

where v_{th} is the thermal velocity, E_{fn_t} and E_{fp_t} are the quasi-Fermi levels for trapped electrons and holes, respectively, and E_{μ} is the mobility gap. Using the same approximations the quasi-Fermi levels for trapped charge become

$$E_{fn_t} = E_c + kT \ln\left(\frac{n+p}{N}\right), \quad (6)$$

$$E_{fp_t} = E_v - kT \ln\left(\frac{n+p}{N}\right). \quad (7)$$

Under the listed assumptions the quasi-Fermi levels for trapped charge are located symmetrically around midgap, i.e. the distance between the quasi-Fermi level for trapped electrons and the conduction-band edge is equal to the distance between the quasi-Fermi level for trapped holes and the valence-band edge. Furthermore, the quasi-Fermi level for the majority carriers is approximately equal to the quasi-Fermi level for trapped majority carriers ($|E_{fn_t, p_t} - E_{fn, p}| \leq kT \ln(2)$, where E_{fn_t, p_t} and $E_{fn, p}$ refer to the quasi-Fermi levels for the *majority* carriers). In the following derivation of the activation energy of SRH recombination processes, we make use of the symmetry around midgap by first considering only traps in the upper half of the bandgap ($E_t > E_{\mu}/2$), and then determine the activation energy of traps located in the lower half from the symmetry around midgap.

We approximate Eq. (5) by substituting the expression between brackets on the right with 1, when $E_t \leq E_{fn_t}$ and $\exp[(E_{fn_t} - E_t)/kT]$, for $E_t > E_{fn_t}$. Equation (5) then becomes

$$\eta_R(E_t) = \begin{cases} v_{th} \sigma \frac{np}{n+p}, & E_t \leq E_{fn_t} \\ v_{th} \sigma \frac{np}{n+p} \cdot \exp\left(\frac{E_{fn_t} - E_t}{kT}\right), & E_t > E_{fn_t}. \end{cases} \quad (8)$$

The thermal velocity and the effective density of states in the bands are temperature dependent. The thermal velocity follows the following temperature dependent relation:⁸

$$v_{th} = \sqrt{\frac{3kT}{m_e^*}}, \quad (9)$$

where m_e^* is the effective electron mass. The effective density of states as a function of temperature can be written as⁸

$$N = N_{T_0} \left(\frac{T}{T_0}\right)^{3/2}, \quad (10)$$

where N_{T_0} is the effective density of states at temperature T_0 . Substitution of Eqs. (9) and (10) in Eq. (8) and rearranging terms gives

$$\eta_R(E_t) = \begin{cases} \sqrt{\frac{3k}{m_e^* T_0^3}} \sigma T^2 \frac{\tilde{n}\tilde{p}}{\tilde{n} + \tilde{p}}, & E \leq E_{fn_t} \\ \sqrt{\frac{3k}{m_e^* T_0^3}} \sigma T^2 \frac{\tilde{n}\tilde{p}}{\tilde{n} + \tilde{p}} \cdot \exp\left(\frac{E_{fn_t} - E_t}{kT}\right), & E_t > E_{fn_t}, \end{cases} \quad (11)$$

where $\tilde{n}$ and $\tilde{p}$ are the electron and hole concentrations, respectively, where we take temperature independent effective density of states [i.e., we substitute the temperature dependent N with the temperature independent N_{T_0} in Eqs. (2) and (3)].

We define the thermal activation energy of a quantity X as

$$E_a = - \frac{\partial [\ln(X[(kT)^{-1}])]}{\partial [(kT)^{-1}]} \quad (12)$$

The term $np/(n+p)$ in the expressions for the recombination efficiency is approximately equal to the minority carrier concentration when $n \gg p$ and when $p \gg n$. Therefore, this term reflects that the recombination efficiency is limited by the least available carrier and thus its activation energy equals the activation energy of the minority carrier concentration, E_a^m . The activation energy of the minority carrier concentration is equal to the maximum energy distance of either quasi-Fermi level with its respective band. We write

$$E_a^m \equiv \begin{cases} E_{fp} - E_v & n \gg p \\ E_c - E_{fn} & n < p. \end{cases} \quad (13)$$

When there is no minority carrier (i.e., $n \approx p$), $np/(n+p)$ reduces to approximately half of either carrier concentration. Note that also in this case Eq. (13) holds as in then the activation energies of both electrons and holes are approximately equal.

Applying Eq. (12) to the remaining terms of Eq. (11) we obtain for the activation energy of the recombination efficiency,

$$E_a^R(E_t) = \begin{cases} E_a^m + 2kT, & E_t \leq E_{fn_t} \\ E_a^m + 2kT - E_{fn_t} + E_t, & E_t > E_{fn_t}, \end{cases} \quad (14)$$

where the term $2kT$ reflects the temperature dependencies of the thermal velocity and the effective density of states.

Finally, we use the symmetry argument to derive the activation energy of the recombination efficiency of traps located in the lower half of the bandgap and obtain

$$E_a^R(E_t) = \begin{cases} E_a^m + E_{fp_t} - E_t + 2kT, & E_t < E_{fp_t} \\ E_a^m + 2kT, & E_{fp_t} \leq E_t \leq E_{fn_t} \\ E_a^m - E_{fn_t} + E_t + 2kT, & E_t > E_{fn_t}. \end{cases} \quad (15)$$

We recall that the quasi-Fermi levels for trapped charge are located symmetrically around midgap and the quasi-Fermi level for the majority carriers is approximately equal to the quasi-Fermi level for trapped majority carriers. Using this result we can approximate Eq. (15) as

$$E_a^R(E_t) \approx \begin{cases} -\Delta E_{fnp} + E_c - E_t + 2kT, & E_t < E_{fp_t} \\ E_a^m + 2kT, & E_{fp_t} \leq E_t \leq E_{fn_t} \\ E_\mu - \Delta E_{fnp} + E_t - E_c + 2kT, & E_t > E_{fn_t}, \end{cases} \quad (16)$$

where ΔE_{fnp} is the separation between quasi-Fermi levels ($E_{fn} - E_{fp}$). The relation in Eq. (16) is illustrated in Fig. 1. Outside the energy range between the quasi-Fermi levels for trapped charge, the activation energy increases linearly toward the band edges and the activation energy at the band edges is equal to $E_\mu - \Delta E_{fnp} + 2kT$.

B. Activation energy of a *p-i-n* device

For the derivation of an analytical expression of the activation energy of a *p-i-n* device we make the additional

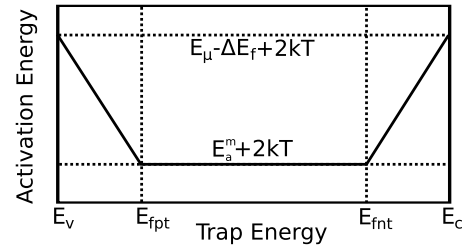


FIG. 1. Activation energy of recombination processes as a function of trap energy.

approximations that the separation between the quasi-Fermi levels is equal to the applied voltage V and the quasi-Fermi levels are constant in the device with respect to the potentials at the contacts. Furthermore, we assume that the electric field in the device is uniform. With these assumptions, we can draw a schematic band diagram, as is shown in Fig. 2(a). As the electric field and the quasi-Fermi levels are constant, the separations between the quasi-Fermi levels and their respective bands become linear functions of position. We can therefore write for the carrier concentrations in the intrinsic layer,

$$n = n_0 \exp \left[- \frac{E_0(x - x_0)}{kT} \right], \quad (17)$$

$$p = p_0 \exp \left[\frac{E_0(x - x_0)}{kT} \right], \quad (18)$$

where E_0 is the uniform electric field in the intrinsic layer, n_0 and p_0 are the electron and hole concentrations, respectively, at position x_0 in the intrinsic layer. For convenience we define x_0 such that $n_0 = p_0$. From Eq. (5) it can be seen that the recombination efficiency scales with the term $np/(n+p)$. In Fig. 2(b) the term $np/(n+p)$ is schematically shown as a function of position in the *p-i-n* device. Using Eqs. (17) and (18) and substituting $n_0 = p_0$, we can write

$$\frac{np}{n+p} = \frac{n_0}{\exp \left[\frac{E_0(x - x_0)}{kT} \right] + \exp \left[- \frac{E_0(x - x_0)}{kT} \right]}. \quad (19)$$

Equation (19) peaks at x_0 , where the carrier concentrations are equal and decays exponentially in either direction away from x_0 .

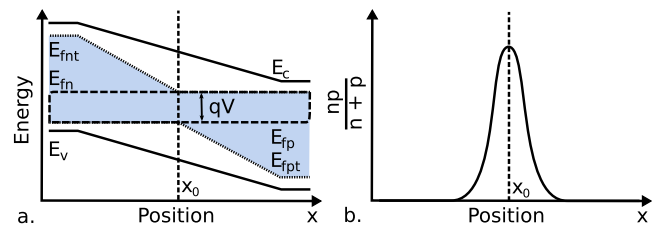


FIG. 2. Schematic band diagram with corresponding term $np/(n+p)$ as a function of position. (a) Schematic band diagram of a *p-i-n* device. Indicated are the voltage V and the quasi-Fermi levels for electrons and holes (E_{fn} and E_{fp} , respectively) and the quasi-Fermi levels for trapped electrons and holes (E_{fnt} and E_{fpt} , respectively). The gray area depicts the energy range between the quasi-Fermi levels for trapped electrons and holes. (b) Schematic figure of the term $np/(n+p)$ as a function of position in the device.

In a first order approximation we assume the recombination takes place between the quasi-Fermi levels for trapped charge (the Taylor and Simmons 0 K approximation⁷). The temperature dependency of the total recombination in the device is obtained by integrating the recombination efficiency over the intrinsic layer. Note, however, that this does not give us the current as we do not take into account the density of states. The integral of Eq. (19) over the intrinsic layer is

$$\begin{aligned} \int_0^W \frac{np}{n+p} dx &= \int_0^W \frac{n_0}{\exp\left[\frac{E_0(x-x_0)}{kT}\right] + \exp\left[\frac{-E_0(x-x_0)}{kT}\right]} dx \\ &= \frac{n_0 kT}{E_0} \left(\arctan \left\{ \exp \left[\frac{E_0(x-x_0)}{kT} \right] \right\} \right)_{x=0}^{x=W} \\ &\approx \frac{n_0 kT}{E_0} \pi. \end{aligned} \quad (20)$$

We first determine the activation energy of the term n_0 . At x_0 the quasi-Fermi levels are located symmetrically around midgap. As the separation of the quasi-Fermi levels is equal to V , it follows that $E_a^m = (E_\mu - V)/2$. Thus, using Eq. (16), the activation energy of n_0 is equal to

$$E_a^R = E_a^m + 2kT = \frac{E_\mu - V}{2} + 2kT. \quad (21)$$

Using Eq. (12) the activation energy of the expression obtained in Eq. (20) then becomes

$$E_a^{p-i-n} = \frac{E_\mu - V}{2} + 3kT. \quad (22)$$

Our assumption that the electric field is uniform in the device is not very realistic. In practice band bending at the p - i and the i - n interface result in a reduction in the electric field in the middle of the device. However, the recombination is highest where $n \approx p$, which naturally leads to a space charge close to zero. Therefore the electric field actually is fairly uniform in the most relevant part of the integral in Eq. (20), and thus the dark current activation energy is not very sensitive to the nonuniform electric field distribution in the device.

By applying the inverse of Eq. (12) to Eq. (22) we find that the current as a function of voltage and temperature is proportional to

$$J \propto T^3 \exp\left(\frac{V - E_\mu}{2kT}\right), \quad (23)$$

which corresponds to the diode equation with an ideality factor of 2. It is well known that the ideality factor of a -Si:H and μc -Si:H devices is, in general, smaller than 2. There are several explanations of this effect. According to Berkel *et al.*,⁶ the energy distribution of traps influences the ideality factor when the number of traps between the quasi-Fermi levels for trapped charge varies strongly with the applied voltage. He attributes ideality factors less than 2 in a -Si:H p - i - n diodes to this voltage dependency of the number active recombination centers. However, this effect on the ideality

factor is independent of temperature and therefore will not affect the slope of dark current activation energy versus the voltage. From this slope we can thus determine a “thermal-ideality factor.” We therefore ascribe differences between the thermal-ideality factor and the ideality factor determined from J - V characteristics to a voltage dependency of the number of active recombination centers.

Also spatial effects may lead to an ideality factor less than 2. The activation energy of recombination processes in a p - i - n device depends on the activation energy of the minority carrier concentration. This activation energy is not constant through the device. As a consequence the dark current activation energy, and thus also the ideality factor, depends on the spatial distribution of the recombination rate.^{9,10} The effect of the spatial variation in the activation energy of the minority carrier concentration is taken into account in the integral of Eq. (20), leading to a difference of kT between Eqs. (21) and (22). However, as the integral in Eq. (20) is over the recombination efficiency, this result is only valid as long as the spatial variation in defect density is small compared to the spatial variation in recombination efficiency. In the case of a highly inhomogeneous defect state distribution, a significant part of the recombination could take place in a region where $n \neq p$, and hence $E_a^m > (E_\mu - V)/2$. For the extreme case we evaluate the activation energy for recombination at an interface with a doped layer, where the quasi-Fermi level of the majority carriers is pinned. Due to this pinning of the quasi-Fermi level for majority carriers, E_a^m varies linearly with the applied voltage and therefore the slope of the activation energy versus the voltage is -1 for these recombination processes, and hence the thermal-ideality factor for these recombination processes is 1. Similarly, recombination via traps outside the energy range confined by the quasi-Fermi levels for trapped charge leads to changes in the thermal-ideality factor. From Eq. (16) it follows that the thermal-ideality factor for these recombination processes is 1 ($\Delta E_{fnp} = V$). Note that due to the steep band tails in μc -Si:H a significant portion of the tail-state recombination may take place outside the energy range between the quasi-Fermi levels for trapped charge.

The analytical model that was presented in this section is based on many approximations, such as a uniform field, the Taylor and Simmons approximation, the decoupled approach for amphoteric states, etc. Furthermore, both the effect of an inhomogeneous spatial distribution of defect states and recombination via traps outside the energy range confined by the quasi-Fermi levels for trapped charge may play a role in the dark current activation energy of p - i - n devices. In Sec. III we therefore compare the analytical model with a detailed numerical model to verify the approximations for the here investigated μc -Si:H devices. To study the applicability of the approximations further we investigate the influence on the dark current activation energy of tail-state recombination or the presence of a defect-rich or amorphous interface layer. However, before we discuss numerical simulations we present in Sec. II C experimental results for μc -Si:H solar cells of which we determine the mobility gap using the dark current activation energy.

C. Experimental

In order to measure the current through a $\mu\text{c-Si:H}$ solar cell accurately at low bias voltages, it is important to prevent current spreading.¹¹ This is achieved by removing the silicon in the surroundings of the contacts, leaving patterned solar cells. The $\mu\text{c-Si:H}$ solar cells consisted of a glass substrate covered with ZnO, a 15–20 nm $\mu\text{c-Si:H}$ *p*-layer, a 1.15 μm $\mu\text{c-Si:H}$ intrinsic layer, and a 15–20 nm *a-Si:H* *n*-layer. Based on previous results we estimate the crystalline volume fraction of the intrinsic layer to be around 60%.¹⁵ The back contact and reflector consists of a ZnO(80 nm)/Al(300 nm)/Cr(50 nm) stack. After deposition of the cells the ZnO of the back contact layer stack was etched around the metal contacts in a HCl solution: During this step the Cr layer prevented etching of the underlying Al and ZnO. Subsequently the silicon layer stack was removed using reactive ion etching. The solar cell parameters for the etched solar cell are an efficiency of 7.2%, a short-circuit current density of 20.8 mA cm⁻², an open-circuit voltage of 0.49 V, and a fill factor of 72%.

We measured the dark current of the cells at 289, 298, 308, and 323 K. In Figs. 3(a) and 3(b) typical dark *J-V* characteristics at different temperatures are shown of two patterned cells, cell 1 [Fig. 3(a)] and cell 2 [Fig. 3(b)]. Cell 2 still shows a shunt resistance for bias voltages below 0.25 V at a temperature of 289 K. The origin of this shunt resistance is not clear, however, the effect of the shunt resistance on the *J-V* characteristics becomes less pronounced at higher temperatures. Thus, we conclude that the thermal activation energy of this shunt is lower than the activation energy of the exponential current voltage relation that dominates the current at bias voltages above 0.25 V. Figure 3(c) shows the dark current activation energy for the two cells. The low activation energy of the shunt resistance of cell 2 has a large effect on the activation energy at voltages below 0.25 V. The dark current activation energy of the cells without shunt resistance follows the predicted linear voltage dependency for low forward bias voltages (between 0 and 0.3 V). Using Eq. (22) the mobility gap was determined as 1.19 eV from the dark current activation energy, which is the average mobility gap determined on the interval from 0 to 0.3 V. In Fig. 3(c) the expression from Eq. (22) is plotted for the extracted mobility gap of 1.19 eV, which also shows that the slope of the activation energy versus voltage is -0.5 from 0 to 0.3 V, and thus the thermal-ideality factor is 2. In comparison, the ideality factor of the *J-V* characteristics in the same voltage range is 1.6, which shows that the ideality factor indeed is affected by the number of active recombination centers. Furthermore, the thermal-ideality factor of 2 in this voltage range suggests that Eq. (22) is valid as for these forward bias voltages there is no indication of a significant influence of tail-state recombination or the presence of a defect-rich or amorphous interface layer on the dark current activation energy.

D. Discussion of the obtained mobility gap

From the dark current activation energy of $\mu\text{c-Si:H}$ *p-i-n* devices, we determined the mobility gap of the intrinsic

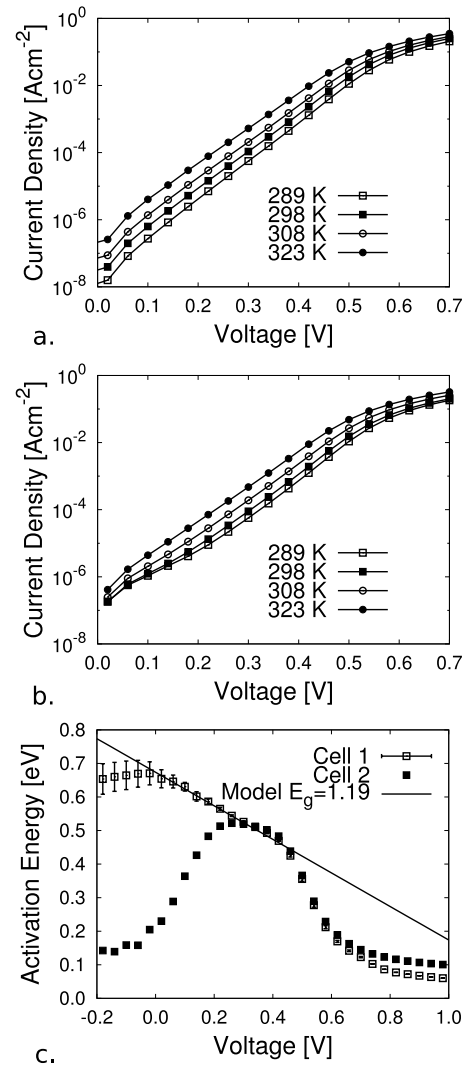


FIG. 3. The characteristics of the prepared isolated solar cells. (a) The dark *J-V* characteristics of cell 1, a cell without shunt resistance, at 289, 298, 308, and 323 K. (b) The dark *J-V* characteristics of cell 2, a cell with shunt resistance, at 290, 298, 309, and 323 K. (c) The activation energy of cells 1 and 2 as a function of bias voltage. The analytical model from Eq. (22) is plotted for a mobility gap of 1.19 eV.

layer as 1.19 eV. Xu *et al.*⁴ carried out internal photoemission measurements to determine band offsets between *p*-type $\mu\text{c-Si:H}$ and *a-Si:H* and found a mobility gap for $\mu\text{c-Si:H}$ of 1.59 eV for a crystalline volume fraction of 80%. Hamma *et al.*⁵ determined the mobility gap of $\mu\text{c-Si:H}$ using *in situ* contact potential measurements combined with dark conductivity activation energy measurements and found mobility gaps of 1.48 and 1.55 eV for material with crystalline fractions of 70% and 30%, respectively. Xu *et al.*⁴ explained the difference between the mobility gap of $\mu\text{c-Si:H}$ and the bandgap of crystalline silicon with quantum-size effects. However, Carius *et al.*¹² reported that the optical bandgap of $\mu\text{c-Si:H}$ does not show a large influence of quantum-size effects and is close to the bandgap of crystalline silicon. The here reported value for the mobility gap is therefore more in line with the observed optical properties. The difference of 70 meV between the determined mobility gap and the bandgap of *c-Si* may be caused by quantum confinement, however, it may also be related to the assumption of abrupt

mobility edges. In case the mobility edges are not abrupt, it is expected that the measured mobility gap increases with temperature.¹¹ In the limited temperature range of our experiments we have not observed a strong temperature dependency of the mobility gap [i.e., the Arrhenius plots are linear over the measured temperature range, as indicated by the small error bars in Fig. 3(c) over the relevant voltage range].

III. SIMULATION RESULTS

A. Model parameters

In order to study the dark current activation energy of $\mu\text{c-Si:H}$ *p-i-n* devices in more detail, we carried out numerical simulations using the ASA program.¹³ For the simulations we use the effective medium approximation. For experimental reference results we use the same solar cells as in Sec. II. Apart from the mobility gap, which we already determined, we determine input parameters for our simulations from literature, through physical arguments, or by fitting the simulation results to experimental results.

Effective density of states. We assume that the electronic transport in $\mu\text{c-Si:H}$ predominantly takes place through clusters of crystallites or “percolation paths.”¹⁴ This means that as the current flows through only a fraction of the volume (i.e., the long range clusters of crystallites), only the transport states of this fraction of the material are relevant for electronic transport. The effective density of states should therefore scale with the number and size of the clusters of crystallites making long range connections. For simplicity we will assume that the effective density of states scales linearly with the crystalline volume fraction. For our solar cells we estimate the crystalline volume fraction to be around 60%, based on previous results.¹⁵ We assume that the band structure of the crystallites is similar to the band structure in *c-Si* and take the effective density of states in the crystallites equal to the effective density of states of *c-Si* ($N_c = 2.8 \times 10^{19} \text{ cm}^{-3}$ and $N_v = 1.0 \times 10^{19} \text{ cm}^{-3}$ at 300 K).

Band offsets. As we assume that the band structure of the crystallites is similar to *c-Si*, the band offsets between $\mu\text{c-Si:H}$ and *a-Si:H* should be approximately equal to the band offsets between *c-Si* and *a-Si:H*. Various authors have reported similar values for the band offsets between *c-Si* and *a-Si:H*, where the electron affinity of *c-Si* is approximately 0.15 eV higher than of *a-Si:H*.^{16,17}

Band mobility. Recently, measurements on $\mu\text{c-Si:H}$ thin-film transistors have shown conduction-band mobilities of $50 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$.¹⁸ In general, the hole mobility is found to be about three times lower, and, therefore we assume a hole mobility of $15 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$.

Band tails. We assume exponential band tails. The characteristic energy of the valence-band tail has been determined to be 31 meV.^{19,20} The characteristic energy of the conduction-band tail is 33 meV.²¹ In our simulations we assume for both band tails a characteristic energy of 31 eV. Furthermore, in Refs. 19–22 the slope of the band tails appears to be temperature independent up to a temperature range of 250–300 K (Ref. 23) [which is not the case for *a-Si:H* (Refs. 24 and 25)]. By lack of evidence we also assume temperature independent band tails for higher tem-

peratures, up to the maximum temperature of our experiments (323 K).

Midgap states. From electron spin resonance (ESR) spectroscopy it has been found that there are two dangling-bond distributions in $\mu\text{c-Si:H}$ with different paramagnetic properties.²⁶ Presumably these two dangling-bond distributions are separated spatially where one distribution is located within the crystallites and the other in the *a-Si:H* tissue at the columnar boundaries.²⁷ The total defect density was found to be in the range of $5 \times 10^{15} - 1 \times 10^{16} \text{ cm}^{-3}$. The exact value for the dangling-bond concentration in our simulations was obtained by fitting simulated solar cell properties to experimentally obtained properties. The total dangling-bond distribution can be considered broad,^{26,27} and therefore we assumed a Gaussian distribution with a standard deviation of 150 meV.

Contacts. At the ZnO/semiconductor contacts we assume an excess charge carrier density of zero, i.e., infinite surface recombination velocity.

Optical simulations were carried out using the semi-coherent model GENPRO3,¹³ taking into account both coherent and incoherent light propagations. The amount of scattering at a rough interface depends on the roughness of the interface and the complex refractive indexes of the materials, as described in Ref. 28. In our simulations we used a rms roughness of 100 nm for the TCO-*p* interface and for the ZnO/Al interface. Scattering at other interfaces is neglected in our simulations. The optical properties of $\mu\text{c-Si:H}$ can be estimated using the effective medium approximation.²⁹ In this approach the refractive index is computed from the refractive indices of the two phases, *a-Si:H* and $\mu\text{c-Si:H}$, and the crystalline volume fraction. Although this method may not be the most accurate for determining the refractive index of the materials used in the solar cell, the method has the advantage that it allows for a flexible variation in the crystalline volume fraction in simulations. In our simulations we used a crystalline volume fraction of 60%.

We fitted simulated solar cell characteristics to experimental results by varying the following parameters: (i) the capture cross sections of charged and neutral dangling bond and tail states, (ii) the density of states at the mobility edges, (iii) the density of defect states, (iv) the activation energy of the *p*-layer, and (v) the series resistance. In order to make this procedure as reliable as possible we fitted the simulations to experimental results simultaneously for the dark and illuminated *J-V* characteristics, the external quantum efficiency (EQE), and the dark current activation energy of the solar cell as a function of bias voltage. The dark current activation energy was determined the same way as in Sec. II, using the same temperatures (289, 298, 308, and 323 K). The EQE was measured and simulated at 0 V.

In Fig. 4 experimental results and simulation results are compared for several solar cell characteristics. To obtain the results in Fig. 4 we set the capture cross sections for neutral dangling-bond states to $3.0 \times 10^{-16} \text{ cm}^2$, and for neutral tail states to $5.0 \times 10^{-16} \text{ cm}^2$. The capture cross sections for charged states are generally larger than for neutral states due to Coulomb attraction between a charged trap and charge carriers with an opposite charge.³⁰ We used a fixed ratio of a

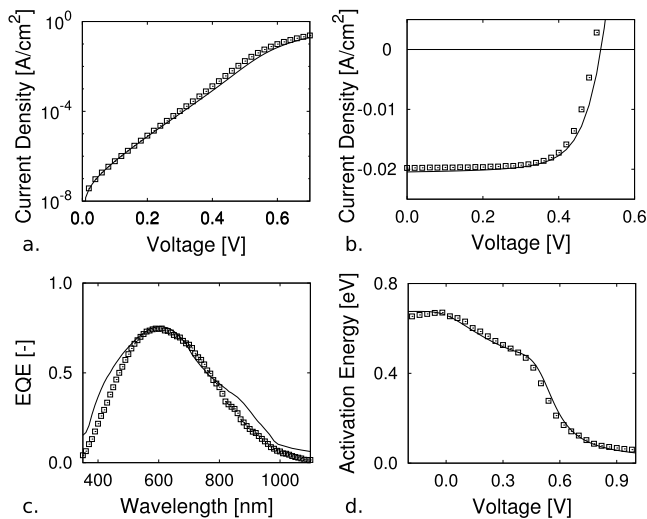


FIG. 4. Measured (symbols) and simulated (lines) solar cell characteristics. (a) The dark J - V characteristics; (b) the illuminated J - V characteristics; (c) the spectral response; (d) the dark current activation energy.

factor of 10 between the capture cross section of charged and neutral states. The factor of 10 has previously been used to model defects in both a -Si:H and μc -Si:H material.³ Other fitted parameters were the density of states at the valence and conduction-band mobility edges were set to 1.04×10^{20} and $2.8 \times 10^{20} \text{ cm}^{-3} \text{ eV}^{-1}$, respectively, the density of dangling bonds was set to $5.0 \times 10^{15} \text{ cm}^{-3}$, the activation energy of the p -layer was set to 0.15 eV, and we used a series resistance of $0.45 \Omega \text{ cm}^2$ to fit the current density at voltages above 0.5 V. The dark and illuminated J - V characteristics [Figs. 4(a) and 4(b)] both show a close match between measurements and simulations. The simulated short-circuit current density in Fig. 4(b) is slightly too high. In Fig. 4(c) the simulated and measured EQE is shown. The simulated EQE is overall slightly higher than the measured EQE, which corresponds to the too large simulated short-circuit current density. In Fig. 4(d) the simulated and experimental dark current activation energies are shown. It can be seen from Fig. 4(d) that we obtained a good match between simulation and experiment for the dark current activation energy. In Sec. II we determined the mobility gap using Eq. (22) and the dark current activation energy obtained from experiments. Applying the same procedures on the simulated dark current activation energy, we obtain a value for the mobility gap, which should be approximately the same as the mobility gap used in the simulations. We found a mobility gap of 1.17 eV using Eq. (22), compared to 1.19 eV for the mobility gap taken in the simulations. Comparing the analytical approximation of the dark current activation energy with the simulated dark current activation energy we find that the analytical approximation is quite accurate, despite the many approximations made in Sec. II.

B. Influence of band tails on the dark current activation energy

We study the influence of recombination via tail states by distinguishing between current due to tail states and the current due to defect states. The current due to recombination

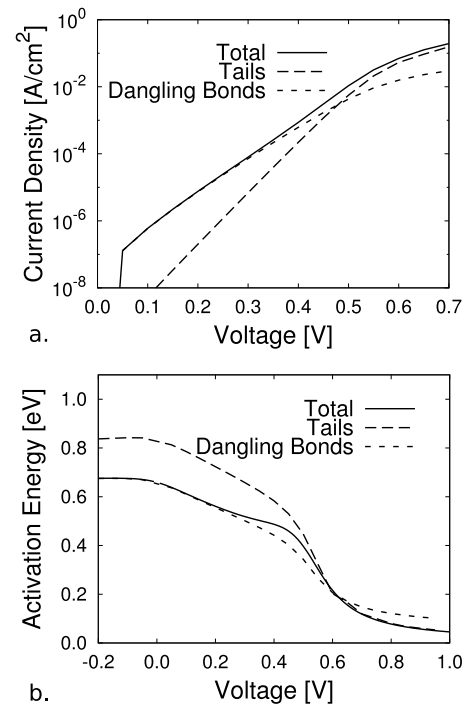


FIG. 5. (a) The tail-recombination current and the dangling-bond-recombination current at 298 K. (b) The thermal activation energy of the tail-recombination current and the dangling-bond-recombination current.

through tail states, the tail recombination current, is determined by integrating the recombination analogous to the integral Eq. (1), where the total recombination is replaced with the recombination via tail states only. Likewise the current due to recombination via dangling-bond states, the dangling-bond recombination current, is determined by integrating the recombination via dangling bonds in the device.

In Fig. 5(a) we show the tail-recombination current density and the dangling-bond recombination current density for a temperature of 298 K. For reference the total simulated current density is also shown. For voltages below 0.3 V the total current density approximately equals the dangling-bond-recombination current density. For higher voltages the tail-recombination current density becomes increasingly important, while at the same time the effects of series resistance and space charge limited current start to play a role. In Fig. 5(b) we show the thermal activation energies of the dangling-bond-recombination current density and the tail-recombination current density. For reference the simulated activation energy of the total current density is also shown in Fig. 5(b). Up to a voltage of 0.3 V the activation energy of the total current density is primarily determined by the activation energy of the dangling-bond-recombination current density. Above 0.3 V the activation energy is partly determined by recombination via tail states and the activation energy does not follow Eq. (22). We can conclude that, together with the effects of series resistance and space charge limited current, recombination via tail states can limit the voltage range for which the dark current activation energy can be used to determine the mobility gap.

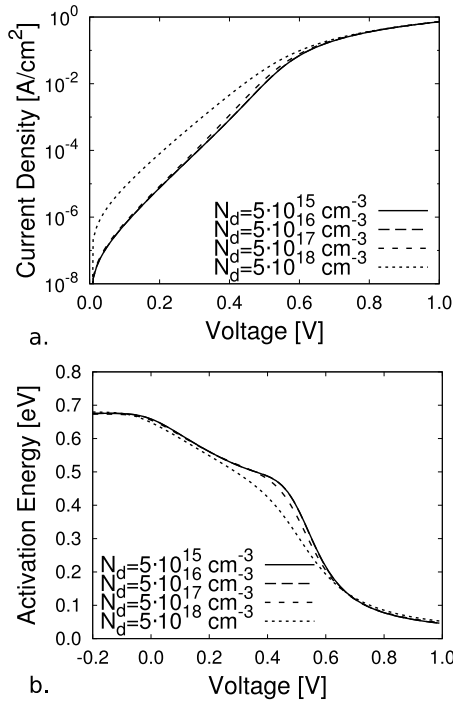


FIG. 6. (a) The dark current density of the $\mu\text{c-Si:H}$ solar cell for various defect densities in a 10 nm thick layer adjacent to the $p-i$ interface. The defect density in the bulk is $5 \times 10^{15} \text{ cm}^{-3}$. (b) The dark current activation energy for the various defect densities in the defect-rich interface.

C. Influence of a defect-rich or amorphous $p-i$ interface on the dark current activation energy

In Fig. 6 we show the influence of a variation in the defect density in a 10 nm thick layer adjacent to the $p-i$ interface on the dark current density [Fig. 6(a)] and the dark current activation energy [Fig. 6(b)]. A defect density of $5 \times 10^{15} \text{ cm}^{-3}$ is equal to the defect density in the rest of the intrinsic layer. When the defect density is varied over several orders of magnitude, the influence on the dark current density and the activation energy is marginal. Figure 6(a) shows that for a defect density of $5 \times 10^{18} \text{ cm}^{-3}$ the dark current density is considerably higher than for a defect density lower or equal to $5 \times 10^{17} \text{ cm}^{-3}$. The mobility gap as evaluated with Eq. (22) from the simulated dark current activation energy was 1.17 eV for a defect density less than $5 \times 10^{18} \text{ cm}^{-3}$. When the defect density in the interface layer is $5 \times 10^{18} \text{ cm}^{-3}$, the mobility gap determined from the simulations is 1.14 eV. The simulations suggest that the value obtained for the mobility gap from the dark current activation energy is not sensitive to the spatial distribution of dangling-bond defects.

We can explain that the dark current activation energy is fairly insensitive to the presence of a highly defective interface layer. For moderately defect-rich interface layers, with a defect density up to $5 \times 10^{17} \text{ cm}^{-3}$, the total recombination rate in the device is dominated by the bulk of the intrinsic layer. As the total recombination rate is dominated by bulk recombination for these defect densities in the interface layer, the current density is not strongly affected by the interface layer, as can be seen from Fig. 6(a). However, for a high defect density in the interface layer ($5 \times 10^{18} \text{ cm}^{-3}$) the

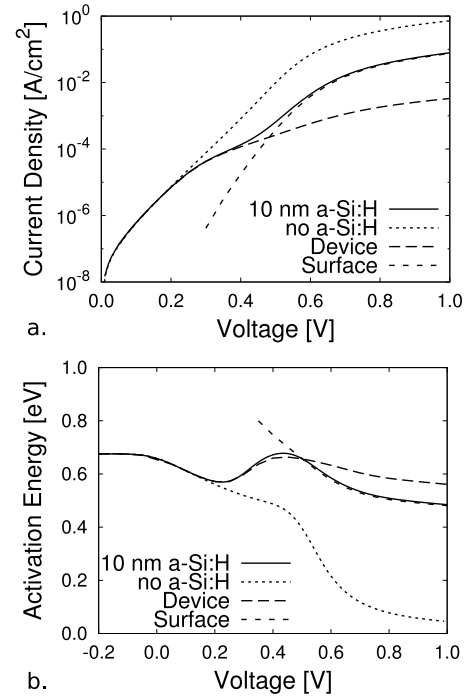


FIG. 7. (a) The dark current density of the $\mu\text{c-Si:H}$ solar cells with and without a 10 nm thick $a\text{-Si:H}$ layer adjacent to the $p-i$ interface. For the solar cell with an $a\text{-Si:H}$ layer the current density computed as the integral of the recombination over the device (without surface recombination) is also shown. The difference between the recombination current density and the total current density is the current arising from surface recombination. (b) The dark current activation energy for a solar cell with and without a 10 nm thick $a\text{-Si:H}$ layer adjacent to the $p-i$ interface. For the solar cell with an $a\text{-Si:H}$ layer the dark current activation energy of the recombination in the device and the activation energy of the surface recombination current are also shown.

simulated current density in Fig. 6(a) is significantly higher than for the lower defect densities. The recombination-rate profile (not shown) shows that this increase in current density can be attributed to a high recombination rate in the defect-rich interface layer. However, from the band diagrams (not shown) it follows that in this case there is strong band bending in the interface region. At the recombination peak in the interface layer, the strong band bending leads to quasi-Fermi levels which are located approximately symmetrically around midgap, despite the proximity of the $p-i$ interface. Thus the activation energy of the total recombination rate is not strongly affected by the introduction of a defect-rich interface layer.

In some cases an amorphous incubation layer is formed during the initial growth of a $\mu\text{c-Si:H}$ layer.^{31,32} We investigated the influence of such an incubation layer by inserting a 10 nm thick $a\text{-Si:H}$ layer between the p -layer and the $\mu\text{c-Si:H}$ intrinsic layer. Figure 7(a) shows the dark current density of a $\mu\text{c-Si:H}$ solar cell with $a\text{-Si:H}$ incubation layer and without. The current density is the same up to 0.15 V for the solar cells with $a\text{-Si:H}$ interface layer and without. Above 0.15 V the current density through the cell with an amorphous interface layer is considerably lower than without. Similar to Sec. II we integrated the recombination in the device according to Eq. (1). However, this time we integrated the total recombination rate in the device, excluding surface recombination at the contacts (which is not computed

explicitly in ASA). The thus obtained device-recombination current is shown in Fig. 7(a). For voltages above 0.35 V there is an increasing difference between the device-recombination current density and the total simulated current density, showing that there is a large contribution of the surface recombination at the contacts. The surface recombination current density can be computed as the difference between the total current density and the device-recombination current density and is also shown in Fig. 7(a).

The influence of the amorphous interface layer between the p -layer and the μc -Si:H intrinsic layer can be explained as follows: The valence-band offset between a -Si:H and μc -Si:H is rather large (0.41 eV) and inhibits the injection of holes from the p -layer into the intrinsic layer. For a 10 nm thick a -Si:H incubation layer the limitations on the injection of holes becomes prominent above 0.15 V. As a result the hole concentration (not shown) and thus the recombination rate in the intrinsic layer are reduced, resulting in a relatively larger contribution of surface recombination and recombination in the p -layer. Note that we have assumed infinite recombination velocities at the contacts. However, we verified with simulations that the overall effect on the current density of reducing recombination velocities is small. The simulations (not shown) indicate that reducing recombination velocities at the contacts leads to higher minority carrier concentrations in the defect-rich doped layers, effectively moving the recombination from the contact surfaces to the volume of the doped layers.

Figure 7(b) shows the dark current activation energy of the solar cells with and without a -Si:H interface layer and the activation energy of the device-recombination current and of the surface recombination current. It can be seen that Eq. (22) is not valid as the slope of the voltage-dependent dark current activation energy is only -0.5 in the voltage range of 0–0.15 V. The simulations suggest that an incubation layer of 10 nm prevents a straightforward determination of the mobility gap. It should be noted that, for thin a -Si:H incubation layers, tunneling of holes through the incubation layer may reduce the influence of the amorphous layer on the dark current.

IV. CONCLUSIONS

We derived an analytical model for the dark current activation energy of μc -Si:H p - i - n devices and showed that this dark current activation energy can be used to determine the mobility gap of the intrinsic layer in the device. Using this method we found a mobility gap of 1.19 eV. This is in line with findings of Brammer *et al.*³ and Carius *et al.*¹² but considerably lower than the reported values of 1.59 and 1.48 eV for crystalline fractions of 30% and 70%, respectively.⁵

As the analytical model is based on many approximations, we compared the analytical model with detailed numerical simulations. The results show that, in the case of a μc -Si:H solar cell, the analytical model provides an accurate description of the dark current activation energy for voltages below 0.3 V.

The method is further investigated using numerical

simulations in order to evaluate the reliability of the method and the applicability of the method on other than the investigated device. The numerical simulations indicate that the method can still be used for devices which show the influence of recombination via tail states and recombination in a defect-rich interface layer at the p - i interface. However, tail-state recombination may limit the voltage range for which the analytical model is valid. We also tested the influence of an a -Si:H incubation layer. An a -Si:H incubation layer may lead to a non-neglectable contribution of surface recombination to the dark current density, impeding a straightforward interpretation of the dark current activation energy. Further experimental work is required to investigate the applicability of the method on a wider range of μc -Si:H and a -Si:H devices.

ACKNOWLEDGMENTS

The authors would like to thank Franz Birmans, Rebekka van Aubel, Kah-Yoong Chan, and Thomas Kirchartz.

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