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2009

Carrier Drift-Mobilities and Solar Cell Models for Amorphous and Nanocrystalline Silicon

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Carrier drift-mobilities and solar cell models for amorphous and nanocrystalline silicon

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ABSTRACT

Hole drift mobilities in hydrogenated amorphous silicon (a-Si:H) and nanocrystalline silicon (nc-Si:H) are in the range of 10^{-3} to 1 cm^2/Vs at room-temperature. These low drift mobilities establish corresponding hole mobility limits to the power generation and useful thicknesses of the solar cells. The properties of as-deposited a-Si:H *nip* solar cells are quite close to their hole mobility limit, but the corresponding limit has not been examined for nc-Si:H solar cells. We explore the predictions for nc-Si:H solar cells based on parameters and values estimated from hole drift-mobility and related measurements. The indicate that the hole mobility limit for nc-Si:H cells corresponds to an optimum intrinsic-layer thickness of 2-3 μm, whereas the best nc-Si:H solar cells (10% conversion efficiency) have thicknesses around 2 μm.

INTRODUCTION

The mobility μ of a charge carrier describes its drift-velocity v in the presence of an electric field F: $v = \mu F$. Mobilities are significant in solar cells because they affect the useful thickness of the layer of material that absorbs the sunlight. For crystalline solar cells, this thickness is typically that of the "ambipolar diffusion length":

$$L_{amb} = \sqrt{2(kT/e)\mu\tau_R} \quad ,$$ (1)

where μ is the mobility of the minority carrier (holes in *n*-type material), and τ_R is its recombination lifetime [1]. In crystalline silicon, the hole mobility of about 500 cm^2/Vs and a recombination lifetime of about 100 microseconds yield a diffusion length of 500 μm.

Many materials that are interesting for solar cells have much lower carrier mobilities, and much shorter recombination lifetimes, than are typical for crystalline silicon. Under the conditions present in solar cells, holes in hydrogenated amorphous silicon (a-Si:H) have drift mobilities more than 10^5 smaller than in c-Si, and recombination lifetimes about 10^2 smaller. The corresponding ambipolar diffusion lengths are around 0.1 μm.

The absorber layers in a-Si:H can be several times thicker than this. The reason that this extra thickness is useful is that, for low-mobility solar cells, the *space-charge* layer near the junction of the cell also makes a significant contribution. In c-Si the space-charge layer is the depletion region, whose width is determined by the dopant density. In a-Si:H and in other low-mobility, highly insulating materials, the width of the space-charge layer L_{SC} is determined directly by the carrier mobilities and the photocarrier generation rate G [2]. Holes drift so slowly in such materials that the space-charge from slowly drifting holes screens the built-in potential, thus limiting the width of the region from which holes can be collected. Denoting the limiting drift mobility as μ_p, the expression for the width of this region is [2]:

$$L_{SC} = (\Delta V)^{1/2}\left(\frac{4\mu_p\varepsilon\varepsilon_0}{eG}\right)^{1/4} \quad ,$$ (2)

where ΔV is the electrostatic potential dropped across the space-charge layer and $\varepsilon\varepsilon_0$ is the

dielectric constant of the layer. This expression is based on the minimal "5-parameter" model for a semiconductor layer described below.

In Fig. 1 we illustrate the ambipolar diffusion length and the space-charge width as a function of the hole mobility μ_p; we assume a uniform photogeneration rate $G = 10^{21}$ cm^{-3}s^{-1} (for calculating L_{SC}) and recombination lifetime $\tau_R = 10^{-6}$ s (for L_{amb}). The voltage dropped across the space-charge width is 1.0 V, which is a nominal value similar to the built-in potentials and open-circuit voltages for silicon-based solar cells.

The figure also indicates the corresponding lengths for c-Si, for which the diffusion length is very much larger than the depletion-width. The regime for c-Si, in which the diffusion length is dominant, is well known and is the basis for most semiconductor device physics texts. However, when the mobility less than 1 cm^2/Vs, the space-charge width is larger than the diffusion length. This is the regime applicable to amorphous silicon, for which the hole drift-mobility is less than 10^{-2} cm^2/Vs; we expect the same regime to apply with many organic, polymeric, and nanostructured hybrid materials.

In this paper we elaborate on the "mobility perspective" for hydrogenated amorphous silicon and nanocrystalline silicon (nc-Si:H) solar cells. In the next section we review a relatively simple device model that has been proposed for as-deposited amorphous silicon solar cells [3,4]; there are about seven essential electronic parameters, and with conventional estimates for their values, the model describes the solar cells well. Of the seven parameters, those determining the hole drift mobility have a significance exceeded only by the bandgap itself. We next propose a set of values for the same minimal parameter set that apply to nanocrystalline silicon (the material formerly known as microcrystalline silicon). The values for the parameters are not as well established as for a-Si:H; additionally, nc-Si:H lies at the boundary of space-charge and diffusion domination, so the mobility parameters are not as dominant as for a-Si:H. Nonetheless, the mobility perspective offers an interesting perspective on the cells. With the present choices of values, it predicts an optimum thickness (2-3 µm) and a voltage (0.60-0.64 V) that are somewhat larger than the values for optimized cells (2 µm, 0.60 V).

Fig. 1: Ambipolar diffusion length and space-charge width as a function of carrier mobility for the "5-parameter" model of a low-mobility semiconductor. The associated generation rate and recombination lifetime are $G = 10^{21}$ cm^{-3}s^{-1} and $\tau_r = 10^{-6}$ s; the voltage dropped across the space-charge width is 1.0 V. The markers on the right axis indicate corresponding lengths for c-Si assuming $\tau_r = 10^{-4}$ s and a doping level 10^{16} cm^{-3}. Based on ref. [2].

MODELING a-Si:H CELLS WITH A MINIMAL PARAMETER SET

Six electronic parameters seem to be the minimum required for modeling any semiconductor layer used in a solar cell; these parameters are listed in the unshaded lines in Table 1. We shall refer to this model as the "5-parameter" model because the larger of the carrier mobilities usually has no significant effect on its predictions. This model has been developed at some length elsewhere [2,5, 6], and may be
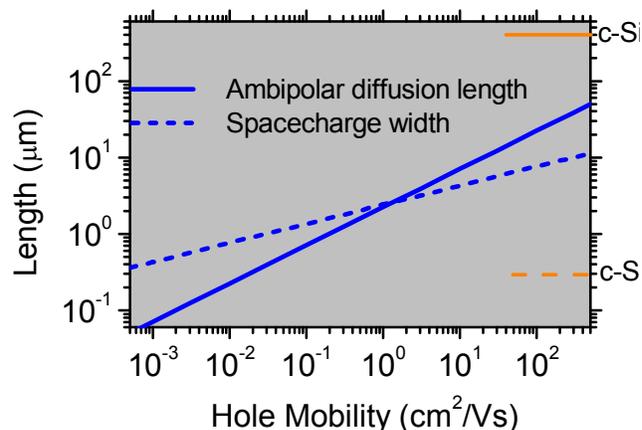
directly useful in some materials [7]. For a-Si:H, we think that two additional parameters are required to give a good account of as-deposited cells (before light-soaking is significant). The first is the width of the exponential tail of the valence band ΔE_V, which is usually just called the valence bandtail width. The second parameter is the coefficient b_T describing trapping of a density of mobile holes p onto a density of bandtail traps N_t ($dp/dt = -b_T pN_T$) . The recombination coefficient b_R describes recombination of a density of electrons n onto a density of holes N_T^+ trapped in the

Table 1: Parameter values for a-Si:H solar cell modeling (from ref. [3]).	
Parameter	*Value*
Bandgap E_G	1.74 eV
Band mobilities μ_p^0 (holes) and μ_n (electrons)	0.3 cm^2/Vs 2.0
Band densities-of-states N_V and N_C	4x10^{20} cm^{-3} 4x10^{20}
Recombination coefficient b_R	10^{-9} cm^{3}s^{-1}
Valence bandtail width ΔE_V	0.04 eV
Hole trapping coefficient b_T	1.6x10^{-9} cm^{3}s^{-1}
Defect density	unused

valence bandtail ($dn/dt = -b_R nN_T^+$).Deep levels, usually identified as dangling bonds, are not included in the model; they do need to be incorporated to model the light-soaked state of a-Si:H cells.

We shall refer to this model as the "7-parameter" model for a-Si:H, as originally proposed by Zhu, *et al.* [3]; although the parameter count is apparently 8, the electron drift-mobility is so much larger than the hole drift-mobility that it is inconsequential in practice. Because we shall shortly extend this model to nanocrystalline silicon, we note its additional assumptions. First, the valence bandedge at E_V is assumed to lie within the exponential valence bandtail; this viewpoint is consistent with the interpretation of drift-mobility measurements, and most workers believe that E_V marks a "mobility edge" separating localized trap states and delocalized transport states. This assumption sets the value for the density of bandtail traps g_V^0 at E_V (see Appendix 1). Second, the conduction bandtail is neglected; at about 22 meV [8], the conduction bandtail in a-Si:H is sufficiently narrow that this neglect is justified near room-temperature. The assumption should be reassessed for work at low temperatures below about 225 K or for a-SiGe:H alloys, which have broader conduction bandtails [9]. Recombination of free holes with electrons is also neglected.

The 7-parameter model is motivated by general arguments [2, 5, 6] that the space-charge of slowly drifting holes is likely to
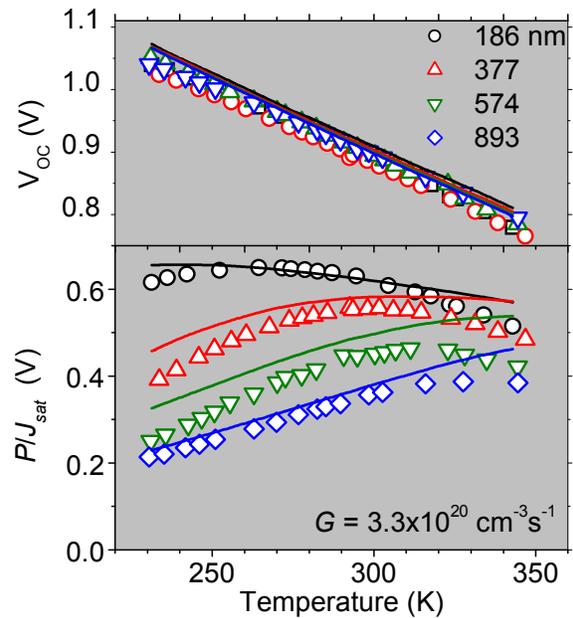

Fig. 2: a-Si:H solar cell parameters for four cells measured at varying temperatures. The symbols indicate measurements with near infrared laser illumination on cells prepared at United Solar Ovonic LLC. The curves are calculations of the "hole mobility limit" based on the parameters in Table 1. Based on ref. [4].

dominate a-Si:H solar cells. The values for the modeling parameters were chosen for consistency with hole drift-mobility measurements. We think that it is important for solar cell models of low-mobility semiconductors to be constrained this way. To facilitate such constraints, in Appendix 1 we give the expressions for calculating the drift-mobility based on the values of the bandtail parameters; the calculations can then be checked for consistency with the experimental results. Electron and hole drift-mobilities for a-Si:H and related materials have been reviewed fairly recently [8].

For a-Si:H, the 7-parameter model has been tested by comparing its predictions with the temperature-dependent properties of *nip* cells of varying thickness; the results are presented in Fig. 2 [4]. The cells were made at United Solar Ovonic, LLC, and they did not incorporate a back reflector or a textured substrate; the optoelectronic properties of the cells should be comparable to the optimized, high-efficiency cells made by United Solar. For the measurements, intense near-infrared laser illumination was used instead of solar simulator illumination; since the laser is nearly uniformly absorbed in the intrinsic layer, this procedure simplifies the photogeneration profile compared to that obtained with solar illumination while maintaining a similar photocurrent. We think that the comparison with uniformly absorbed illumination is more stringent than a comparison of the power vs. thickness relation using solar illumination; the solar spectrum contains a significant component that is absorbed close to the *p/i* interface, and hardly tests the electronic properties of the a-Si:H. The calculations were done using the the AMPS 1D program (Pennsylvania State University®) and the parameter values of Table 1. The *p* and *n* layers were given ideal properties; as intended, the details of these have no noticeable effect on the calculations.

We consider the agreement of calculation and measurement to be very good, noting also that the values for the modeling parameters were published before these measurements were made, and that this same parameter set also accounts well for the power-thickness relation for similar cells under solar illumination [10].

What can such device modeling teach us? One lesson from the model is that the hole drift-mobility is indeed central to the properties of a-Si:H solar cells. In Fig. 3 we present three plots of the calculated power from a solar cell as a function of the absorber layer thickness; the lowest plot used the same parameters as Fig. 2. As can be seen, the power from a-Si:H cells saturates for absorber layer thicknesses greater than about 300 nm, which is our estimate for the useful thickness of the as-deposited cell. If one could increase the hole band mobility tenfold, the calculations show that the power output would rise markedly for thicker cells, and that the useful thickness rises to about 600 nm.
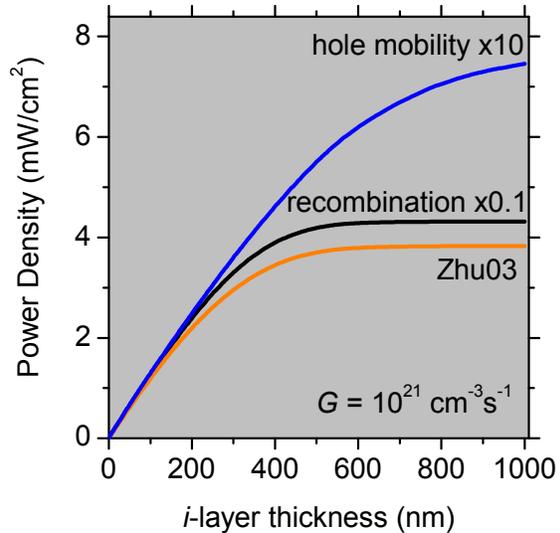

Fig. 3: Model calculations for the power density from *pin* solar cells with a uniform photogeneration rate in the intrinsic layer. The curve labeled Zhu03 uses the parameter valaues from Table 1. The other curves indicate the results after increasing μ_p^0 tenfold, or reducing b_R tenfold.

This behavior is due to the increase in the width L_{SC} of the space-charge region, and is qualitatively consistent with the behavior expected from eq. (2). It should be noted that texturing and back reflectors modify the power-thickness relation, which then shows a weak maximum instead of smooth saturation [11].

On the other hand, if we reduce the recombination coefficient tenfold, there is a smaller increase, presumably due to the increased ambipolar diffusion length. The fact that mobility has a larger effect on the cell's power than its recombination coefficient is the "recombination paradox" of low-mobility solar cells. On the one hand, the substantial fraction of photogenerated carriers that do not contribute to the cell's photocurrent are recombining somewhere in the cell; on the other hand, the parameters of this recombination have little effect on the power. In effect, recombination establishes an absorbing boundary to the space-charge region; the width of the space-charge region itself is mainly dictated by the hole mobility.

HOLE MOBILITY LIMIT FOR NANOCRYSTALLINE SILICON SOLAR CELLS

In this section we propose values for the parameter set of Table 1 that are useful as a starting point for understanding two aspects of nanocrystalline silicon solar cells: the best open-circuit voltages of about 0.6 V [12], and the typical thickness of the most efficient cells, which is about two microns [13,14]. A series of modeling studies on nc-Si:H solar cells has been published by a Kolkata-Palaiseau collaboration ([15] and further references therein), and there has been a recent paper from a Jülich-Delft collaboration [16]. These papers treat several important issues for nc-Si:H cells that we leave untouched here, where we are primarily trying to establish fundamental limits to the performance of these cells. They generally use more parameters and more intricate models than we have. More importantly, the values for the bandtail parameters vary noticeably. In Appendix 1 we present a procedure for checking these values for consistency with hole drift-mobility measurements. The set of parameter values in the present work was constrained to be consistent with these measurements, and we hope that the procedure in Appendix 1 will assist other modelers to do the same.

Table 2 presents our proposed parameters values. The three fundamental electronic parameters, E_G, N_V, and N_C are given the same values as for c-Si. In their recent study, Pieters, *et al.* [16], have made a similar proposal; their measurements on dark currents suggest a slightly increased value $E_G = 1.17$ eV. In Table 2, the valence bandtail width $\Delta E_V = 30$ meV and the hole mobility band parameter $\mu_p^0 = 0.7$ cm^2/Vs are set directly from hole drift-mobility experiments on cells from Forschungszentrum Jülich [17]. It is interesting that the value for the hole band mobility μ_p^0 is essentially the same as for a-Si:H, which suggests that transport in these nc-Si:H materials also occurs at a mobility-edge [8]. The reduced valence bandtail width in nc-Si:H compared to a-Si:H seems reasonable.

In Table 2, the bandtail trapping coefficient b_T is markedly lower in nc-Si:H than in a-Si:H. The associated

Table 2: Parameters for nc-Si:H solar cell modeling.	
Parameter	*Value*
Bandgap E_G	1.12 eV
Band mobilities μ_p^0 (holes) and μ_n (electrons)	0.7 cm^2/Vs [17] 3.0 [18]
Band densities-of-states N_V and N_C	1x10^{19} cm^{-3} 2.8x10^{19}
Recombination coefficient b_R	10^{-10}-10^{-9} cm^{3}s^{-1} [20,21]
Valence bandtail width ΔE_V	0.03 eV [17]
Hole trapping coefficient b_T	1.0x10^{-10} cm^{3}s^{-1}
Defect density	unused

fitting parameter from hole drift-mobility measurements is the bandtail trap emission frequency prefactor v, which is connected to b_T through the detailed balance expression $v = N_V b_T$. v is about 10^9 s^{-1} in nc-Si:H, which is about 10^3 times smaller than in a-Si:H [17]. About a factor 40 of this reduction in v is expected from detailed balance and from the reduced value for N_V compared to a-Si:H; the reduction in b_T is the unexplained remainder. Schiff has proposed that this reduction is a manifestation of "Meyer-Neldel" behavior for bandtail trap emission in a-Si:H and nc-Si:H [19].

The bandtail recombination coefficient b_R has been estimated from transient measurements on photogenerated space-charge layers by Juška, *et al.* [20,21] using nc-Si:H diodes from Université de Neuchâtel and Prague. Their method seems well suited to determining the recombination parameter for solar cell modeling; the values of b_R varied from $10^{-9} - 10^{-10}$ cm^{3}s^{-1}.

Several groups have measured the ambipolar diffusion length L_{amb} in nc-Si:H films using the steady-state photocarrier grating (SSPG) method; the largest values are about 300 nm [22,23,24]. This value is much smaller than expected from the parameters of Table 2; the procedure for calculating L_{amb} is presented in Appendix 2. As the original authors suggested, the recombination traffic of electrons and holes is probably passing through defect levels instead of the valence bandtail.

As for a-Si:H, we neglect the conduction bandtails and equate the electron band mobility with the measured drift-mobility [18]. Unlike the situation for a-Si:H, the conduction bandtail width has not been extensively studied in nc-Si:H. The assumption that its breadth remains negligible near room-temperature does appear consistent with transient photocurrent measurements by Reynolds, *et al.* [25].

The 7-parameter model is simple enough that an analytical expression for the open-circuit voltage is available. Presuming ideal n and p layers and spatially uniform photogeneration G [2],

$$eV_{OC} = E_G + \frac{kT}{2}\left\{\ln\left(\frac{G}{b_R N_C^2}\right) + 2\ln\left(\frac{G}{b_T N_V^2}\right)\right\} - \frac{(kT)^2}{2\Delta E_V}\ln\left[\frac{b_R}{b_T}\left(\frac{G}{b_T N_V^2}\right)\right] \tag{3}$$

The results are presented as Fig. 4, which also incorporates the temperature-dependent bandgap [26]; we neglected the temperature-dependences of N_V and N_C. For a-Si:H, the calculation is consistent with the measurements in Fig. 2. The generation rate G corresponds to a short-circuit current from a 1 micron cell of 16 mA/cm^2, which is comparable to the values reported for solar illumination with nc-Si:H cells. The recombination lifetime due to bandtail recombination is $(b_R G)^{-1/2}$. With the range of values from Table 2, the lifetime evaluates as 1-3 μs, which is several times longer than some experimental estimates for recombination lifetimes in nc-Si:H diodes [27]. Fig. 4 shows a range of V_{OC} from 0.60-0.64 V at 298 K, depending on the value of b_R; the results agree fairly well with the largest open-circuit voltages of about 0.60 V for nc-Si:H solar cells [12]. To the best of our knowledge, the temperature dependence of V_{OC} for these high V_{OC} cells has not been reported; Fig. 4 corresponds to a predicted value dV_{OC}/dT ranging from -1.3 meV/K to -1.4 meV/K near 298 K.

In Fig. 5 we present the power as a function of the intrinsic layer thickness for the a-Si:H and the nc-Si:H models. The a-Si:H model, which suggests a useful thickness of about 300 nm for as-deposited cells, is in good agreement with measurements [4]. The nc-Si:H model indicates a useful thickness of 2-3 μm. This is somewhat larger than the thicknesses of high efficiency nc-Si:H cells (9.8%, 2.0 μm thickness, FF= 0.70 [13] and 9.9%, 1.8 μm thickness, FF=0.74 [14]). These best efficiencies are from nc-Si:H cells with lower values of V_{OC} of about 0.55 V

CONCLUSIONS

The best nc-Si:H solar cells are close to the limit due to fundamental hole transport and recombination processes involving the valence bandtail. We refer to this limit as "the hole mobility limit"; as valence bandtails are improved, most likely by narrowing, hole transport will improve (by diminished trapping). While b_R is not very consequential in a-Si:H modeling (cf. Fig. 3), it affects the model results for nc-Si:H noticeably, and additional measurements on materials more similar to those used for current, optimized cells would be valuable. It is worth noting that the fundamental physics that determines b_R is not well established. The fact that optimized cells are somewhat thinner than the present hole mobility limit calculation needs further research.

If the model and parameter choices prove to be correct in essence, one possibility for the difference between realized cells and the calculation would be that nc-Si:H layers become coarser grained and more defective for positions that are further from the substrate. However, contemporary deposition technology reduces this problem by modifying the growth conditions during the growth process to maintain a homogeneous material throughout [28]. Furthermore, the hole drift mobility measurements on which the present model was based were done on cells with intrinsic layers thicker than 3 μm [17]. At present, deterioration of the electronic quality of the nc-Si:H for thicker layers can't be established as the mechanism that determines the 2 μm thickness for optimized cells.

A second mechanism would involve defects, which may play a comparable role in recombination and transport to the bandtails. This possibility can't be excluded, but it isn't very satisfactory to rely on a coincidence that two supposedly independent physical features – the bandtail and the defect density – compete fairly evenly for hole trapping and recombination.
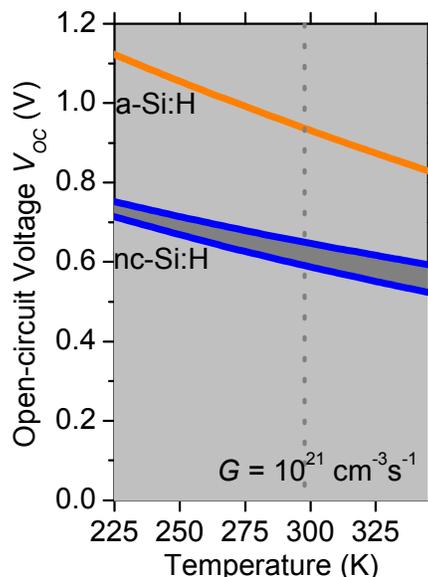

Fig. 4: Open-circuit voltage calculated as a function of temperature from eq. (3) using the parameter values of Table 1 (for a-Si:H) and Table 2 (for nc-Si:H, and including a range of values for b_R).
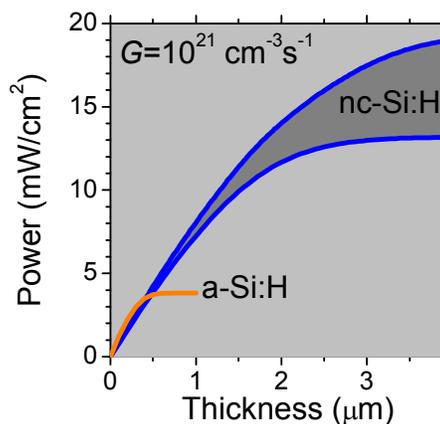

Fig. 5: Predictions of the power output of *pin* solar cells for varying intrinsic-layer thickness at room temperature. The photogeneration rate G in the intrinsic layer is uniform throughout the layer. The model is based on the parameter values of Table 1 (a-Si:H) and Table 2 (nc-Si:H, including a range of values for b_R).

ACKNOWLEDGMENTS

APPENDIX 1: CONNECTING SOLAR CELL MODELS TO DRIFT MOBILITY MEASUREMENTS

Drift-mobilities established using the time-of-flight technique are somewhat tricky to interpret in materials that exhibit "anomalously dispersive" transport. The drift-mobility is defined as:

$$\mu_D = \frac{L}{Ft_T} \; , \tag{4}$$

where L is the mean displacement of the photocarriers following their photogeneration [29], t_T is the "transit time" corresponding to this displacement, and F is the electric field used for the measurement. In practice, for samples exhibiting dispersive transport, μ_D depends noticeably on the thickness of sample used for the measurement, and there is also a dependence on the magnitude of the electric field that (misleadingly) suggests nonlinear transport. These effects reflect the fact that the mean displacement of a carrier $L(t)$ following its photogeneration at time $t = 0$ is sublinear in time:

$$L(t) \propto Ft^\alpha \; ,$$

where α is called the "dispersion parameter". In the presence of dispersion, it is necessary to compare the drift-mobilities of differing materials and differing experiments at some specific value of the ratio L/F [9]; we have generally adopted $L/F = 2\times10^{-9}$ cm^2/Vs for our work on a-Si:H, but this value can be too small for convenient work with higher mobility materials.

In amorphous and nanocrystalline silicon, dispersive behavior is a usually a consequence of trapping by a bandtail of states. For an exponential valence bandtail, the "multiple-trapping" model for the drift-mobility of holes yields (see Appendix 2):

$$\mu_D(T) = \left(N_V b_T \left(L/F\right)\right)^{1-\frac{1}{\alpha}} \left(\mu_p^0 \frac{N_V}{kTg_V^0} \frac{\sin(\alpha\pi)}{\alpha\pi}\right)^{\frac{1}{\alpha}} \quad \left(\mu_D < \mu_V^0\right) , \tag{5}$$

where (L/F) is the ratio of the hole displacement L to the electric field F in the drift-mobility experiment, kT is the thermal energy, $\alpha = kT/\Delta E_V$ is the dispersion parameter, and g_V^0 is the bandtail density-of-states evaluated at E_V. The expression applies for temperatures such that $\mu_D < \mu_V^0$; at higher temperatures $\mu_D = \mu_V^0$.

The parameter g_V^0 is the factor governing the density of valence bandtail traps $g_V(E) = g_V^0 \exp\left(-(E - E_V)/\Delta E_V\right)$. While it does not appear in Tables 1 and 2, it is commonly specified in solar cell modeling. The approach we have taken is to assume that the valence bandedge E_V lies within the exponential bandtail, in which case one can derive the equation relating it to the effective density-of-states N_V [2]:

$$\frac{N_V}{\Delta E_V g_V^0} = \frac{\alpha}{1-\alpha} \quad . \tag{6}$$

If E_V does not lie in the bandtail, the band mobility parameter fitted to time-of-flight measurements at low temperatures ($kT < \Delta E_V$) would be smaller than the drift mobility measured at high temperatures; this possibility can be excluded for electrons in a-Si:H [8].

Equation (5) is unambiguous for calculating the drift-mobility at a specified temperature. To calculate the temperature-dependent drift-mobility, we presume that g_V^0 and b_T are temperature-independent, and that the temperature-dependence of N_V follows eq. (6):

$$\frac{N_V(T)}{N_V^0} = \frac{\alpha(1-\alpha_0)}{\alpha_0(1-\alpha)} \quad ,$$

where N_V^0 is the value of N_V at a reference temperature T_0 (presumably room temperature), and $\alpha_0 = kT_0/\Delta E_V$. We obtain [30]:

$$\mu_D(T) = \left[\frac{\alpha(1-\alpha_0)}{\alpha_0(1-\alpha)}\right]\left(N_V^0 b_T \left(L/F\right)\right)^{1-1/\alpha}\left(\mu_p^0 \frac{N_V^0}{kTg_V^0}\frac{\sin(\alpha\pi)}{\alpha\pi}\right)^{1/\alpha} \quad . \tag{7}$$

In Fig. 6 we compare one set of measurements on a-Si:H (Dinca, *et al.*, [31]) with the corresponding mobilities calculated using the three different sets of parameter values of Table 1. The curve identified as Zhu03 corresponds to Table 1, for which the parameter values were intentionally matched to the hole drift-mobility measurements. Both of the other parameter sets have poor agreement with the hole drift-mobility, despite the fact that no single parameter value is unreasonable; the parameter values are typical of modeling papers that don't explicitly check for consistency with hole drift measurements. Efforts to use the set of values "B" for solar cell modeling lead to cell power-thickness functions that are inferior to actual a-Si:H cells. Efforts to use the set of values "A" lead to power-thickness relations that are superior to real cells, but the difficulty is masked in practice because it is usually compensated by defects.
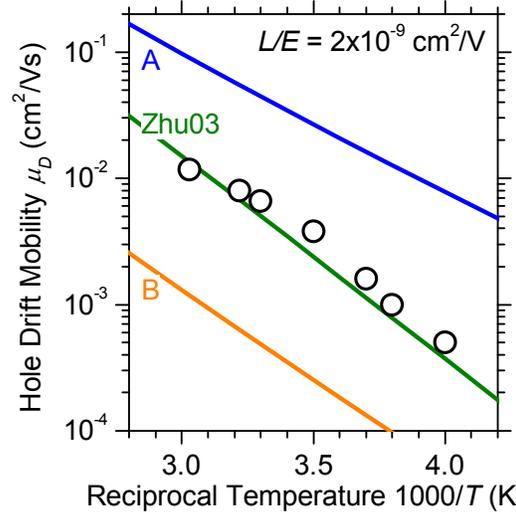

Fig. 6: The symbols indicate hole drift-mobility measurements on a BP Solar cell as reported by Dinca, *et al.* [31]. The smooth curves are the predictions using bandtail parameter values from Table 3.

Table 3: Bandtail parameter proposals for a-Si:H			
Parameter	Zhu03[3]	A	B
Band mobility μ_p^0 (cm^2/Vs)	0.3	5.0	0.3
Band densities-of-states N_V (295 K)	4×10^{20}	1.0×10^{20}	2.5×10^{20}
Valence bandtail width ΔE_V (eV)	0.040	0.047	0.048
Trapping coefficient b_T (cm^{3}s^{-1})	1.6×10^{-9}	3×10^{-10}	7×10^{-9}
Trap density g_V^0 at E_V (cm^{-3}eV^{-1})	6×10^{21}	4×10^{21}	1.0×10^{22}

APPENDIX 2: CONNECTING THE 7-PARAMETER MODEL WITH STEADY-STATE PHOTOCARRIER GRATING MEASUREMENTS

For the model of Tables 1 and 2, which does not incorporate either defects or conduction bandtail trapping, the ambipolar diffusion length L_{amb} can be calculated as follows. For a field-free region, the model predicts a recombination time $\tau_R = 1/\sqrt{Gb_R}$. The bandtail multiple-trapping expression for the drift L_{drift} of a hole distribution following its photogeneration at time $t = 0$ is obtained by integrating eq. (6) in [32] with respect to time:

$$L_{drift}(t) = F\left(\mu_h^0/(N_V b_T)\right)\left(\frac{N_V}{kTg_V^0}\frac{\sin(\alpha\pi)}{\alpha\pi}\right)(N_V b_T t)^\alpha , \tag{8}$$

where F is the electric field; we have also used the detailed balance relation $\nu = b_T N_V$. Eq. (8) is the fundamental equation from which eq. (5) is obtained; for a given value of L_{drift}/F, one solves for the corresponding "transit time" t_T, and then uses the fundamental definition for the drift mobility in eq. (4).

There is a "generalized Einstein relation" connecting this drift with diffusion of a carrier [33]; the root-mean-square width L_D of an initially narrow distribution is related to L_{drift} as:

$$(L_D(t))^2 = (kT/e)(L_{drift}(t)/F) , \tag{8}$$

where e is the electronic charge.

Ambipolar diffusion involves the spreading of an initially narrow distribution with equal densities of both charges of photocarrier. If one carrier is much more mobile than the other, the details of its drift properties are unimportant, and the ambipolar diffusion length can be written as:

$$L_{amb} = \sqrt{2}L_D(\tau_R) = \left\{(2kT/e)(L_{drift}(\tau_R)/F)\right\}^{1/2} . \tag{9}$$

Gu, *et al.* [33] reported that this prediction agreed fairly well with measurements for a-Si:H, which is thus an experimental confirmation of the generalized Einstein relation.

For $G = 10^{21}$ cm^{-3} and $b_R = 10^{-10}$ cm^{3}s^{-1}, the recombination time is 3.1 μs. Using the parameter values of Table 2, the ambipolar diffusion length is 2.5 μm at room temperature and is thus very close to the useful thickness of Fig. 5.

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29. Most experimental papers cited here calculate the drift-mobility assuming that the mean displacement L at the transit-time is half the sample thickness d ($L = d /2$) [9]. Some experimenters use the older expression $L = d$ (cf. [18]), which yields mobilities that are twice as large.

30. This expression in square brackets differs slightly from eq. (4) of ref. [8] because that reference implicitly assumed that the product $N_V b_T$ is temperature-independent. This assumption requires that the temperature-dependence of b_T compensates that of N_V, which seems arbitrary. The fittings to drift-mobilities are not substantially affected; this can be seen in Fig. 6, where the fitting Zhu03 seems satisfactory with the original parameters.

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