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# THERMIONIC EMISSION MODEL FOR INTERFACE EFFECTS ON THE OPEN-CIRCUIT VOLTAGE OF AMORPHOUS SILICON BASED SOLAR CELLS

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## ABSTRACT

We present computer modeling for effects of the *p/i* interface upon the open-circuit voltage $V_{OC}$ in amorphous silicon based *pin* solar cells. We show that the modeling is consistent with measurements on the intensity-dependence for the interface effect, and we present an interpretation for the modeling based on thermionic emission of electrons over the electrostatic barrier at the *p/i* interface. We present additional modeling of the relation of $V_{OC}$ with the intrinsic layer bandgap $E_G$. The experimental correlation for optimized cells is $V_{OC} = (E_G/e)$-0.79. The correlation is simply explained if $V_{OC}$ in these cells is determined by the intrinsic layer, and in particular by the (variable) bandgap and by a non-varying valence bandtail width (about 48 meV) of this layer.

## INTRODUCTION

In Fig. 1 we have illustrated results on the correlation of $V_{OC}$ with the bandgap of the intrinsic layer for amorphous silicon based, *pin* solar cells from United Solar Systems Corp. [1-5]. We also illustrate a fitting line $V_{OC} = (E_G/e) - 0.79$ V. The data are strongly biased – they represent the best, "optimized" cells obtainable at a particular time. The span of devices represented in this figure is enormous. The intrinsic layers included germanium-silicon alloys deposited under quite variable conditions.

It is thus remarkable that the correlation is so simple. The correlation also gains significance because $V_{OC}$ varies rather little with the thickness of the intrinsic layer or with the state of light-soaking of the sample.

The simple correlation $V_{OC} = (E_G/e) - 0.79$ V demands an equally simple explanation. Such an explanation would also permit us to assess whether present values of $V_{OC}$ might be improved by further optimization of these cells. The fact that the slope of the linear fitting to $V_{OC}$ vs. $E_G/e$ is unity suggests that, for these cells, there is relatively little influence of the doped layers and interfaces on $V_{OC}$; one may say that these cells have reached the *intrinsic limit* where $V_{OC}$ is determined by the properties of the intrinsic layer. It further appears that the offset of 0.79 V is determined by the width of the exponential bandtail of the valence band. This valence bandtail width doesn't vary much with bandgap, and is reported to be 48 meV in several experiments with a-Si:H and a-SiGe:H [6,7].

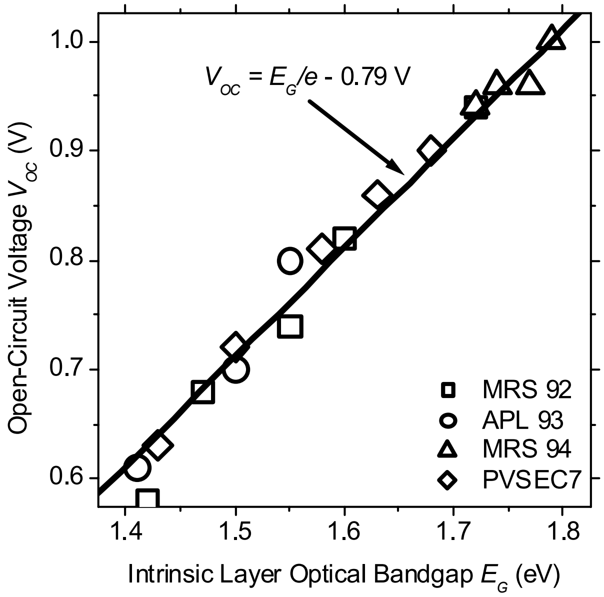

Fig. 1: Correlation of the open-circuit voltage with the optical bandgap for a-Si:H and a-SiGe:H based solar cells. MRS92-[3], PVSEC7-[4], MRS94-[2], APL93-[5].

Objections may be raised to this highly simplified viewpoint, and we are neglecting several well established effects. In this paper we delve into just one of these effects, which is the influence of the *p/i* interface upon $V_{OC}$. Open-circuit voltages lower than those illustrated in Fig. 1 are found in cells with sub-optimal *p/i* interfaces. By modeling these effects, we hope to better understand them and thus to ascertain the extent to which the *p/i* interface is affecting it.

## *p/i* INTERFACE EFFECTS

Perhaps the best-known evidence for significant interface effects upon $V_{OC}$ is the observation that improved *p*-layers and *p/i* interface regions leads to increases in $V_{OC}$ [8,9,10]. This type of information is not, however, well-suited for modeling studies. In recent years, the Pennsylvania State University (PSU) group has

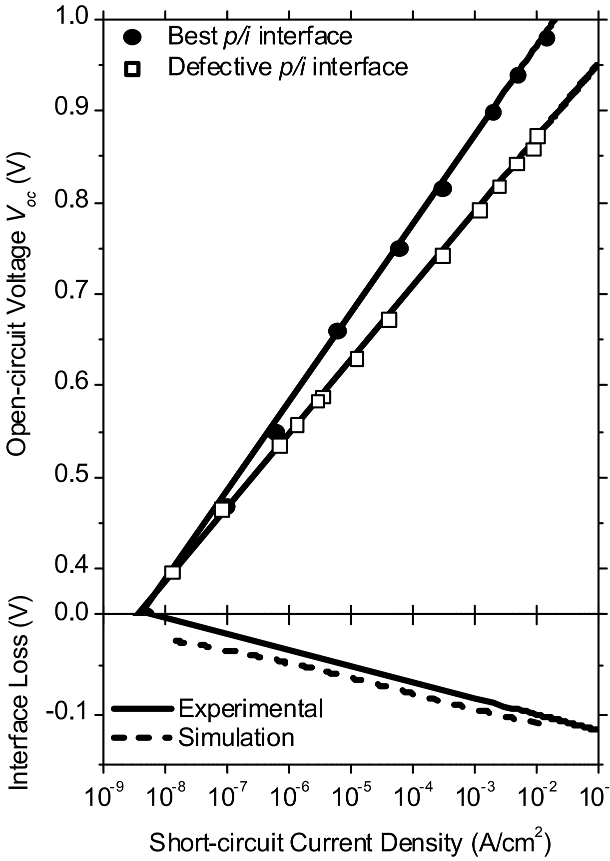

Fig. 2: (*upper*) Open-circuit voltage as a function of white-light intensity for two *pin* cells with comparable i-layers and differing *p*-layers; the short-circuit current $J_{SC}$ is a surrogate for intensity. Solar (AM 1.5) illumination corresponds roughly to $10^{-2}$ A/cm$^2$. After Pearce, *et al.* [11]. (*lower*) Interface effect on $V_{OC}$ as a function of illumination intensity. Experimental data are from the upper panel. The simulation is described in the text, and used a *p*-layer Fermi energy that was 1.43 eV below the conduction bandedge $E_C$ to model the "defective" *p/i* interface.

championed the intensity-dependence of $V_{OC}$ for its sensitivity to interface and light-soaking effects [11].

Some of the PSU measurements are replotted in Fig. 2 (upper panel), which illustrates $V_{OC}$ vs. log($J_{SC}$) for two *pin* solar cells with comparable intrinsic (*i*) layers but different *p/i* interfaces. The difference between the two samples depends only logarithmically upon intensity. It is noteworthy that defective interfaces have a larger effect on $V_{OC}$ for higher intensities. To the best of our knowledge, this fairly simple aspect of interface effects on $V_{OC}$ has not been studied prior to the PSU work, and we don't presently know whether the behavior in Fig. 2 is universal [12].

In the lower panel, the "experimental" line is the difference in the $V_{OC}$ fitting lines for the two samples. The curve labeled "simulation" is based on calculations using the AMPS PC computer program [13]. The intrinsic layer parameters are described elsewhere [14], but we do note here that deep levels (dangling bonds, etc.) were *not* included. $V_{OC}$ was calculated for two *p*-layers (energy gap 1.96 eV) with Fermi energies $E_F$ that were 1.68 eV and 1.43 eV below the conduction bandedge $E_C$ [15]. The larger value of $E_C$-$E_F$ yields a fairly ideal *p*-layer, and for this simulation $V_{OC}$ was close to its intrinsic limit for the entire range of intensities. The lower value is less ideal, and was chosen so that the interface loss in $V_{OC}$ is close to the experimental value at $10^{-2}$ A/cm$^2$. The intensity-dependences of the experimental and simulation curves coincide fairly well without further parameter adjustments.

One difficulty with simulation work is that one can conceive of many different implementations of either the *p/i* interface, and there is very little experimental data with which to constrain the choice of models. It is therefore important to have some idea as to the universality of a behavior such as we have illustrated in Fig. 2. Based on our modeling experiments thus far, it appears that interface loss of $V_{OC}$ is primarily due to thermionic emission of *electrons* from the quasi-Fermi energy in the intrinsic layer, over the barrier at the *p/i* interface, and into the *p*-layer where they immediately recombine [14].

This thermionic emission perspective is helpful because it suggests that most of the interface loss can be attributed to the barrier height which limits the thermionic process. A full description of this viewpoint cannot be given here. In Fig. 3, I have illustrated the profiles for the conduction bandedge $E_C$ and the electron quasi-Fermi level $E_{Fe}$ under open-circuit conditions. The same

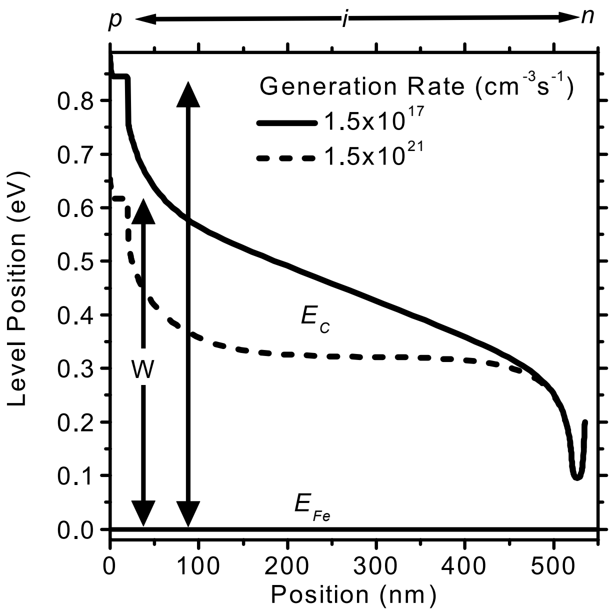

Fig. 3: Calculated profiles for the conduction bandedge $E_C$ and the electron quasi-Fermi level $E_{Fe}$ in a *pin* solar cell under open-circuit conditions. Results are shown for two different illumination intensities. An electron current flows across the *p/i* interface at the left; the current is due to thermionic emission over the barrier *W*.

parameter set was used as for the simulations in Fig. 2. Two different illumination intensities are shown.

For both intensities, the electron quasi-Fermi energy $E_{Fe}$ is essentially constant across the cell. There is nonetheless a current of electrons traveling from right to left across the *p/i* interface. Numerical study of this current density shows that it may be interpreted as thermionic emission over the barrier *W* illustrated in the figure. The exactly matching countercurrent of holes across the *p/i* interface is the origin of interface losses to $V_{OC}$. The fact that the barrier *W* increases strongly as the intensity falls means that the thermionic emission current falls strongly, and this is the fundamental reason that interface losses are lower at lower intensities [16].

## DISCUSSION

In Fig. 4 we illustrate the model predictions for how $V_{OC}$ (under solar illumination) depends on the intrinsic layer bandgap for the two different *p*-layers. The curve labeled “fit to data” is copied from Fig. 1. We first discuss the curve labeled “Simulation (ideal *p/i).*” This simulation used the *p*-layer parameter $E_C$-$E_F$ = 1.68 eV. As the intrinsic layer bandgap shrunk, all of the difference in bandgap between the *p*-layer and the *i*-layer was taken as the conduction bandedge. The assumption that all of the offset is at the conduction bandedge was also taken for the *n*-layer [17]. Interestingly, the slope of the $V_{OC}$ vs. ($E_G$/*e*) line is slightly less than unity for the simulations, and the simulation thus predicts slightly larger values for $V_{OC}$ for lower bandgaps than are measured. In the model, this effect is due to the increase in $J_{SC}$ as the bandgap declines; $V_{OC}$ declines at exactly the same rate as ($E_G$/*e*) if the short-circuit current densities are kept exactly the same.

We thus learn that the unity slope for the experimental correlation of $V_{OC}$ with $E_G$ most likely represents an accidental cancellation of two effects. The first is the increase in $J_{SC}$ as $E_G$ declines, which increases $V_{OC}$ slightly. We speculate that the second, canceling effect is a slight increase in the valence bandtail width as the bandgap is reduced. The present experimental knowledge is inadequate to exclude such a small effect.

We now turn to the “poor *p/i*” simulation, which is based on $E_C$-$E_F$ = 1.43 eV in the *p*-layer. For $E_G$ less than 1.55 eV even this “poor” *p*-layer is effectively ideal. The effects of a poor *p*-layer lead to a significant interface loss in $V_{OC}$ only at larger values of $E_G$.

The only measurements of which we are aware that may be compared with these simulations are the recent ones of Liu and Dalal [18], where $V_{OC}$ was measured for a series of *pin* cells with widely varying intrinsic layer bandgaps, and an intentionally defective *p*-layer. As can be seen in Fig. 4, the measurements are different in their trend from the “poor *p/i*” simulation.

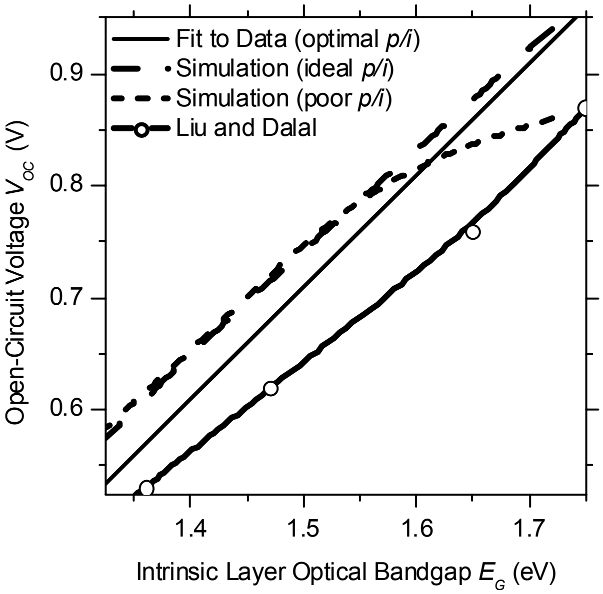

Fig. 4: Open-circuit voltage $V_{OC}$ as a function of optical bandgap. The curve “fit to data” indicates the trend line for optimized cells from several laboratories. The simulations denoted “ideal *p/i*” is affected only by intrinsic layer parameters; only the bandgap was varied for these simulations. The simulation denoted “poor *p/i*” uses the same intrinsic layer parameter but a different *p*-layer parameter set which noticeably affects $V_{OC}$ for larger bandgaps.

This discrepancy should not be overinterpreted; at present, it is unclear whether the simulations need to be modified, or whether the sample series would have reproduced the “optimal” trend line with a better *p*-layer. The discrepancy does indicate the type of experiment that would be conclusive as to the extent of interface effects on the upper, “optimized” $V_{OC}$ vs. $E_G$ line. Such an experiment would include pairs of samples at each bandgap. Each pair would include an optimized cell, with $V_{OC}$ near the upper, “optimal” line, and a second with an intentionally defective *p/i* interface.

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12 Unpublished measurements at Syracuse on cells from BP Solar, Inc. with varying a-SiC:H *p*-layers do show the same characteristics: the difference in $V_{OC}$ for for cells with poor and optimal *p*-layers declines at lower intensities.

13 AMPS PC is a copyright of Pennsylvania State University, and was developed by Stephen Fonash's research group there.

14 L. Jiang, S. Rane, E. A. Schiff, Q. Wang, Q. Yuan, in *Amorphous and Heterogeneous Films – 2000*, edited by H. M. Branz, *et al.* (Materials Research Society, Symp. Proc. Vol. 609, Pittsburgh, 2001), A18.3.1.

15 Some additional parameter information. (i) The intrinsic layer bandgap was 1.8 eV. (ii) The conduction band offset and valence band offsets at the *p/i* interface were each 0.08 eV. (iii) The *p*-layer Fermi energy was "pinned" by a large density of doping levels (Gaussian distribution around $E_F$). (iv) The calculation assumed that there was no back-reflector. (v) The *n*-layer bandgap was 1.80 eV, and $E_F$ in this layer was 0.20 eV below $E_C$.

16 To complete the calculation of the interface loss of $V_{OC}$, one needs the relation between this hole current and the change in the hole quasi-Fermi level $E_{Fh}$ across the *p/i* interface. Unlike the thermionic emission case, no analytical approximation to this relation has been proposed. Such an approximation would be quite enlightening.

17 This assumption that only the conduction bandedge is involved in alloying with Ge is suggested by bandtail widths. The conduction bandtail width broadens markedly with alloying, while the valence bandtail width does not. The issue certainly needs further study.

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