

Analytic approximations for solar cell open circuit voltage, short circuit current and fill factor

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Abstract—For a detailed understanding of solar cell operation and optimization it is necessary to know how the main performance parameters (open circuit voltage, short circuit current and fill factor) depend on material and structural parameters. In this work, we give analytic formulas for the case of solar cells consisting of a single layer absorber, derived from the drift-diffusion model under some simplifying assumptions. We provide insight into the dependency of these parameters on mobility, light intensity, contact workfunctions and recombination coefficients, and we derive simple formulas for limiting cases.

I. INTRODUCTION

The most important parameters characterizing a solar cell are the open circuit voltage V_{oc} , the short circuit current I_{sc} and the fill factor FF . Since the cell efficiency is proportional to the product of these three numbers, optimization of a solar cell can be achieved by increasing any of these. For a detailed understanding of performance limits of solar cells, and for their optimization, it is necessary to have knowledge on the dependency of V_{oc} , I_{sc} and FF on the structural and material related parameters. While I_{sc} can be related intuitively to the total optical generation rate minus recombination losses, a clear connection between V_{oc} , and even more between FF and parameters like mobility, contact properties and recombination constants is more difficult to establish and therefore still object of discussion, in particular for organic based devices [1].

Several analytic formulas for V_{oc} do exist [2], which however are based on empirical device parameters like dark saturation and short circuit current, or on physical models but in idealized situation like homogeneous bulk. Such approaches cannot provide information on the dependence on e.g. contact work functions, which is important for organic solar cells [3]. The usual approach to get insight into the parametric dependence of the different performance parameters is therefore to solve numerically the drift-diffusion equations, and to vary the different model parameters [4]. However, it would be highly desirable to have analytic formulas derived from physics-based models, directly relating material and device structure parameters to V_{oc} , I_{sc} and FF .

II. MODEL AND DISCUSSION

Here we try to derive analytic solutions of the 1D drift-diffusion model for a single layer solar cell with two nonselective contacts as most simple prototype of a solar cell. The simplifications needed to find analytic solutions are: (1) generation rate is spatially constant, (2) contacts are Schottky type with fixed barrier and fixed surface recombination velocity, (3) the

electric field is approximately constant, (4) bulk recombination is negligible. The third assumption implies that densities are moderate, which also means that we can use the Boltzmann approximation. Apart from the constant parameters, the second assumption describes a quite generic device setup, to which also p-i-n device can be mapped to. The fourth assumption seems quite restrictive, however it allows to treat the limiting case of surface recombination controlled behaviour exactly, and we will give also estimates for the bulk recombination parameters needed to make bulk recombination relevant.

A sketch of the band profile in thermodynamic equilibrium, illustrating the simulated structure, is given in Fig. 1.

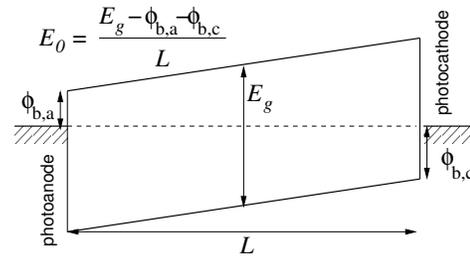


Fig. 1. Schematic bandstructure of the device model at thermodynamic equilibrium. E_g is the band gap, $\phi_{b,a}$ and $\phi_{b,c}$ are the Schottky barriers at the photoanode and -cathode, respectively. E_0 is the electric field at equilibrium, L is the device length.

The model we solve is given by

$$-D_n \nabla^2 n - \mu_n E \nabla n = G \quad (1a)$$

$$-D_p \nabla^2 p + \mu_p E \nabla p = G, \quad (1b)$$

where n and p are the electron and hole densities, $\mu_{n,p}$ the mobilities, $D_{n,p} = k_B T / q \mu_{n,p}$ the diffusion constants and G the generation rate. $E = E_0 - V/L$ is the electric field, which includes the externally applied voltage V . Due to the absence of bulk recombination and the assumption of constant electric field, the two equations decouple and we can consider only e.g. (1a). Equation (1a) is subject to a boundary condition of the form $j_n(0) + GL = j_n(L)$, which expresses the global current continuity. The carrier fluxes at the two contacts are given by [5] $j_n(0) = -v_s[n(0) - n_{0,a}]$ and $j_n(L) = -v_s[n(L) - n_{0,c}]$, where v_s is the contact recombination velocity and $n_{0,a/c}$ are the equilibrium densities at the photoanode and -cathode, given by $n_{0,a} = N_c \exp(-\phi_{b,a}/k_B T)$ and $n_{0,c} = N_c \exp[-(E_g - \phi_{b,c})/k_B T]$.

An analytic solution of (1a) subject to the aforementioned boundary condition can be found as

$$n(x) = n_{0,a} e^{-\frac{qEx}{k_B T}} - \frac{Gx}{\mu_n E} + \frac{\frac{k_B T}{qE} G - v_s \left(n_{0,a} e^{-\frac{qEL}{k_B T}} - n_{0,c} \right)}{\mu_n E + v_s} \quad (2)$$

and similar for the holes. From this solution we calculate the current as (assuming electron-hole symmetry)

$$\begin{aligned} I &= -q[j_n(0) - j_p(0)] \\ &= qGL - \frac{2qv_s}{\mu_n E + v_s} \left\{ \frac{k_B T G}{qE} - \mu_n E \left(n_{0,a} e^{-\frac{qEL}{k_B T}} - n_{0,c} \right) \right\} \end{aligned} \quad (3)$$

While (3) contains all necessary information, it is instructive to look at special cases. In particular, we can distinguish two classes of solutions based on the value of the mobility. The first class corresponds to devices with very low mobilities, as is typically the case in organic materials. In this limit, the current is given by

$$I(V) \approx qGL \left(1 - \frac{2k_B T}{q} \frac{1}{E_g - 2\phi_b - V} \right). \quad (4)$$

The associated open circuit voltage is found to be

$$V_{oc} \approx E_g - 2\phi_b - 2k_B T/q, \quad (5)$$

and therefore depends only on the workfunction difference of the two contacts, while the fill factor is approximately $FF \approx (1 + \gamma - 2\sqrt{\gamma})/(1 - \gamma)$ with $\gamma = (2k_B T/q)/(E_g - 2\phi_b)$.

For the limit of high mobility, on the other hand, the current becomes

$$I(V) \approx qGL - 2qv_s \left(n_{0,a} e^{-\frac{qEL}{k_B T}} - n_{0,c} \right), \quad (6)$$

giving for the open circuit voltage

$$V_{oc} \approx E_g - 2\phi_b - \frac{k_B T}{q} \ln \left(\frac{n_{0,c}}{n_{0,a}} + \frac{GL}{2v_s n_{0,a}} \right). \quad (7)$$

Figure 2 shows the current voltage characteristics under illumination for mobilities ranging from $1000 - 10^{-4} \text{ cm}^2/\text{Vs}$, while all other parameters are fixed. It can be seen that high mobility leads to lower V_{oc} but higher FF , while low mobilities reduce FF but provide considerably higher V_{oc} . The higher V_{oc} can be explained by the fact that with low mobility higher carrier densities and gradients are necessary in order to transport the generated carriers towards the contacts where they recombine, driving the system towards flat band conditions. The higher carrier densities also lead to increased recombination loss at short circuit. For comparison, we give results of numerical drift-diffusion simulations (symbols), showing that only at very low mobility the analytic model starts to deviate systematically from the analytic results, due to charge accumulation near the contacts. We can also notice that crystalline semiconductor solar cells would usually work in the limit of (6), while organic devices would be expected to work in the limit (4).

It is of interest to estimate to what extent the assumption of zero bulk recombination is valid. For this we compare the

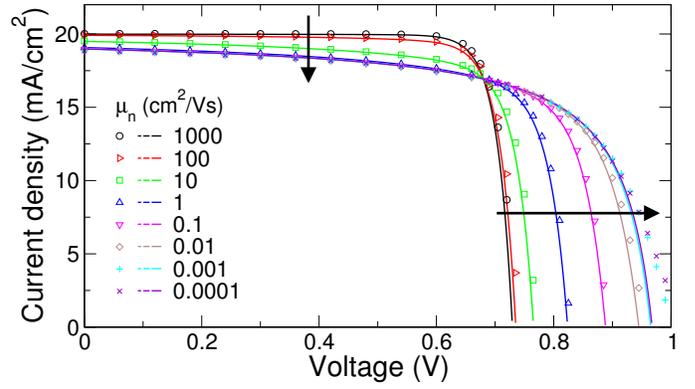


Fig. 2. Current voltage characteristics under illumination for different mobilities. The parameters are: $N_c = 10^{19} \text{ cm}^{-3}$, $E_g = 1.42 \text{ eV}$, $\phi_b = 0.2 \text{ eV}$, $v_s = 10^6 \text{ cm/s}$, $qGL = 20 \text{ mA}$, $L = 100 \text{ nm}$. The symbols give the results of numerical drift-diffusion simulations.

generation rate G with the maximum local recombination rate, which for symmetric parameters is attained at the center of the device ($x = L/2$). Equating generation and recombination provides an estimate of the recombination parameters necessary to make recombination in the bulk relevant compared to recombination at contacts. For the given parameters device

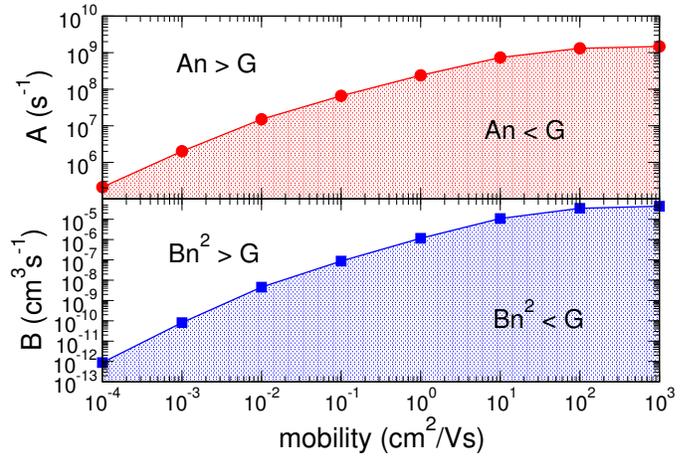


Fig. 3. Recombination parameters required such that Shockley-Read-Hall or direct/bimolecular bulk recombination becomes dominant.

behaviour is mainly controlled by the contact interfaces down to mobilities of around $0.1 - 1 \text{ cm}^2/\text{Vs}$.

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