

Numerical Analysis of Nano-scale Solar Cells with Surface States

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Abstract—As the scale of the solar cell moves into nanometer regime, the numerical analysis should evolve at the same pace. By using the Matlab® as the tool and solving the general Poisson and continuity equations, we are able to have a good platform for the nano-scale solar cells. By adapting proper parameters, the perovskite solar cells and their behavior under different surface recombination conditions were analyzed.

Keywords—*photovoltaic devices, nano-scale devices, numerical simulation, perovskite solar cells*

I. INTRODUCTION

The advances of photovoltaic technology have been impressive in the past few years. One of the promising candidates for the future generation of the solar cells is the nano-scale device which can provide not only smaller footprint but also flexibility on the applications. To simulate these devices, however, will take the ordinary device physics to a different level. The nano-scale calculation of the devices becomes important as the surface states affect the photo-generated carriers much more in these cases. When the concentration of these surface states reaches certain amounts, the Fermi-level of the device will be pinned and thus the carrier collection becomes less efficient. In this work, a numerical method to correlate the surface recombination velocity and the Fermi-level pinning is provided. Also as an example, the lead halide perovskite (CH₃NH₃PbI₃) solar cells in nanometer size can be analyzed in this platform.

II. THEORY

A. General Solver

To properly solve this kind of problem, we adapt the Matlab® platform to enhance the portability of the code and also make the program more user-friendly. The basic physics behind the nano-scale solar cell is pretty much the same as its micron scale predecessor.

The carrier flow caused by the incident solar photons can be described best by the continuity equations[1]:

$$\nabla \cdot J_n = q(U - G) \quad (1)$$

$$\nabla \cdot J_p = q(G - U) \quad (2)$$

, where J_n , J_p are the electron and hole currents, respectively, and G is the generation rate brought by external solar photons, U is the annihilation rate of the generated electron-hole pairs, which is equal to the excess carrier concentration (Δn or Δp)

divided by the carrier lifetime (τ_n or τ_p). With excess carrier generated, the band diagram of the material can be modified by the transport equations [1]:

$$J_n = \mu_n n \nabla E_{fn} \quad (3)$$

$$J_p = \mu_p p \nabla E_{fp} \quad (4)$$

, where μ_n and μ_p are the electron and hole mobility, respectively, and E_{fn} and E_{fp} are the quasi-Fermi level of the device. Finally, the last equation is the Poisson's equation to maintain the charge neutrality[1]:

$$\nabla \cdot (\epsilon(-\nabla V)) = q(p - n + N_d^+ - N_a^-) \quad (5)$$

, where ϵ is the dielectric constant, V is the electrical potential, p , n , N_d^+ , and N_a^- are the hole, electron, the ionized donor, ionized acceptor concentrations, respectively.

To solve these equations, proper boundary conditions are necessary. Since the dimension of the device is small, surface recombination can be an important factor in incorporate. The general consensus is to assume certain recombination velocities at both ends of the device, and thus the derivative of the carrier distribution has to comply with this speed. Other conditions can be found elsewhere [2].

B. Linking Surface Recombination with Bulk recombination

The previous section provides a generic view on solving a solar cell under illumination. However, there are still concerns that the effect of surface states might penetrate into the bulk material. Two methods can be used to accommodate this concerns. The first one is to set up an effective range that extra recombination rate attributed to surface states can be added [1]:

$$U_{sr} \delta_x \approx S_n \times \Delta n \quad (\text{in p-type surface}) \quad (6)$$

$$U_{sr} \delta_x \approx S_p \times \Delta p \quad (\text{in n-type surface}) \quad (7)$$

, where U_{sr} is the effective surface recombination rate, δ_x is a virtually thin layer at the surface, S_n and S_p are the surface recombination velocities for electrons and holes, Δn and Δp are the excess minority carrier concentrations at the surface. This method link the surface recombination with the bulk recombination via the concept that the total recombination rate is $U_{total} = U_{SRH} + U_{sr}$ near the surface and U_{SRH} in the bulk material.

C. Surface Recombination Linked to Fermi-Level Pinning

Another more complicated method is to include the Fermi-level pinning effect when the surface recombination velocity is considered. Taking the regular metal-oxide-semiconductor

interface as the start, the surface traps can pull the Fermi-level and cause additional band bending near the surface. This bending can lead to charge recombination and thus lower the collected photo-generated currents. Additional data for the surface trap details are necessary to calculate such pinning effect and the open-circuit voltage can be greatly modified due to this phenomenon[3].

III. EXAMPLE: PEROVSKITE SOLAR CELLS

Recently, the lead halide perovskite solar cells draws huge attention due their ease of fabrication and high power conversion efficiency(PCE) [4]. The solar cell with PCE close to 20% has been demonstrated[5]. The thin film that was usually synthesized in chemical solution is actually made of multiple grains and surface recombination could be an issue of concerns. As a test of our model, a nano-scale perovskite solar cell was set up for the simulation and the comparison with the published results was made.

The device structure can be seen in Fig. X. In most literatures, the electron and hole transport layers usually do not absorb any photons from solar spectrum, so the main absorption comes from the perovskite layer. As the first test, we set up a simple structure with perovskite layer = 100nm. The detailed parameters of the perovskite material are listed in Table I. With the value of S_n fixed and S_p varied, the photovoltaic I-V characteristics shows different degrees of degradation from V_{oc} , J_{sc} and fill factor, as shown in Fig. 1(b).

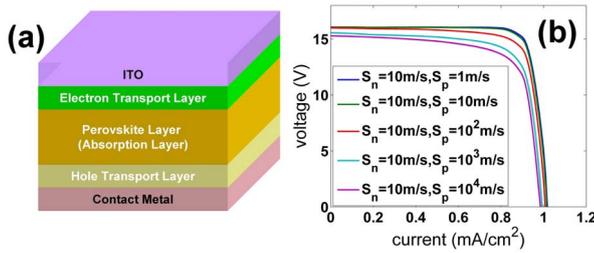


Fig. 1. (a)The schematic diagram of a perovskite thin film solar cell. (b) The photovoltaic I-V curves under different surface recombination velocities of the perovskite solar cell with 100nm absorption layer.

TABLE I. PARAMETERS USED IN THE SIMULATION

Parameters	Typical values	Parameters	Typical values
μ_n	$2 \text{ cm}^2/\text{Vs}$ [6]	N_c	$2.766 \times 10^{24} \text{ m}^{-3}$ [7]
μ_p	$2 \text{ cm}^2/\text{Vs}$ [6]	N_v	$3.917 \times 10^{24} \text{ m}^{-3}$ [7]
E_g	1.55 eV [6]	τ_{srh}	$2.73 \times 10^{-7} \text{ s}$ [6]
χ	3.88 eV [6]	n_i	10^9 cm^{-3} [7]

To compare our results with published data, Burschka et al., reported a perovskite cell with the active layer of 340nm (estimated)[8]. With the parameters in Table I, we were able to calculate the corresponding EQE, IV, band diagram and carrier concentrations, as shown in Fig. 2. From the fitting result, we obtain $V_{oc}=0.94\text{V}$, $J_{sc}=22.82 \text{ mA/cm}^2$, $\text{PCE}=15.11\%$, and $\text{FF}=0.705$. All these numbers are not too far from the measured data: $V_{oc}=0.93\text{V}$, $J_{sc}=20 \text{ mA/cm}^2$, $\text{PCE}=15.11\%$, and $\text{FF}=0.705$.

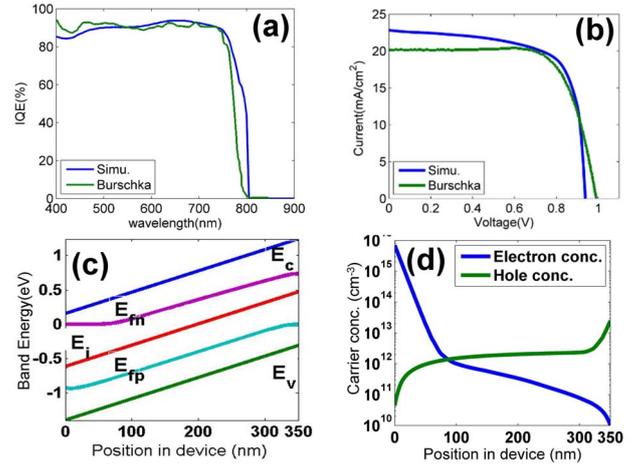


Fig. 2. The calculated and measured perovskite solar cell. (a) EQE, (b) IV under illumination, (c) band diagram, (d) the actual carrier concentration.

IV. CONCLUSION

We demonstrate a Matlab®-based platform to calculate the photovoltaic response of a nano-scale solar cell. Applying the correct material parameters, this program can be used for calculation of the perovskite solar cell with accurate results. We believe this platform should be helpful for the design of the next generation of photovoltaic devices.

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