

How high can fill factor be in organic solar cells?

V.A. Trukhanov, V.V. Bruevich and D.Yu. Paraschuk

Faculty of Physics and International Laser Center, M.V. Lomonosov Moscow State University, Moscow, 119991, Russia

Fundamental limits for efficiency of organic solar cells are actively discussed in comparison with the Shockley-Queisser limit (SQL) calculated for silicon *p-n* junction solar cells [1]. The cell efficiency depends on the form of its current-voltage characteristics characterized by short-circuit current, open-circuit voltage, and fill factor (*FF*). Green calculated a theoretical limit for *FF*, which depends on open-circuit voltage [2,3]. In this work, we show that bilayer organic solar cells can have *FF* exceeding the SQL and discuss the possible reasons of high *FF* in organic solar cells.

Organic solar cells are based on type-II heterojunction: the active layer consists of two organic semiconductors with different electron affinities and ionization potentials, one semiconductor is an electron donor, and the other is electron acceptor. Heterojunction is needed to dissociate excitons formed after light absorption into free charges as excitons in organic materials have a relatively high binding energy and do not dissociate thermally. First organic solar cells were based on planar heterojunction formed by two layers of donor and acceptor [4]. As excitons in organic semiconductors commonly have short diffusion length (~10 nm), not all the excitons reach the heterojunction, dissociate, and contribute to the photocurrent. This limits the efficiency of organic planar heterojunction solar cells. The most efficient organic solar cells are based on bulk heterojunction, in which the active layer is a blend of donor and acceptor materials so that the heterojunction has high surface area, and generation of free charges takes place in the whole volume of the active layer. Nevertheless, the best planar heterojunction solar cells show the efficiency higher than 5% [5], and probably it can be essentially higher for materials with long exciton diffusion length.

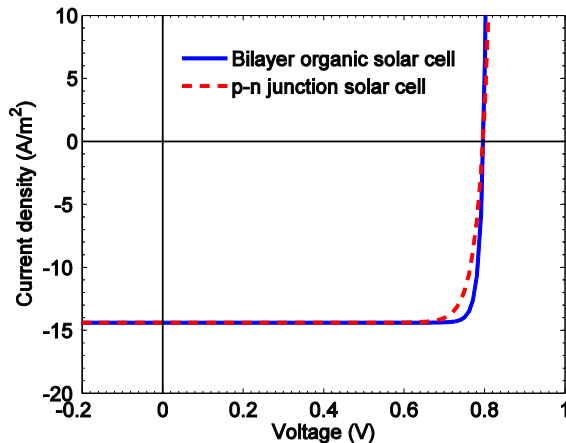


Fig.1. Calculated *J-V* characteristics for a bilayer P3HT:PCBM solar cell (blue solid line) and for an ideal inorganic *p-n* junction solar cell with J_{sc} and V_{oc} the same as for the bilayer organic cell. The current density is calculated for the exciton diffusion length 10 nm in P3HT.

Using a numerical drift-diffusion model, we recently found that planar heterojunction (bilayer) solar cells can have very high FF for the doped active layers [6]. The model accounts for generation, recombination, drift and diffusion of charge carriers, space charge effect in the active layer. Charge generation and recombination in the model depend on the electric field strength at the donor-acceptor interface. Figure 1 shows a calculated current density-voltage (J - V) characteristic of a bilayer organic solar cell (blue solid line) with input parameters for polymer/fullerene (P3HT/PCBM) blend [6] and a doping level of 10^{24} m^{-3} , its FF is 92%.

The textbook model for inorganic p - n junction solar cells gives the following expression for their J - V characteristics:

$$J(V) = J_s \left[\exp\left(\frac{eV}{kT}\right) - 1 \right] - J_{ph} = J_{sc} \left[\frac{\exp(eV/kT) - 1}{\exp(eV_{oc}/kT) - 1} - 1 \right], \quad (1)$$

where J_s and J_{ph} are the saturation current and photocurrent densities, which can be uniquely expressed via the short-circuit current density J_{sc} and V_{oc} ; e is the electron charge, k is the Boltzmann constant, T is the cell temperature. Eq. (1) corresponds to an ideal solar cell with the zero series and infinite shunt resistances and with unity diode ideality factor. The red dashed line in Fig. 1 shows the J - V curve plotted according to Eq. (1) with J_{sc} and V_{oc} the same as for the calculated above bilayer organic solar cell. The FF is 86%, and this is a limit for p - n junction inorganic solar cells at given V_{oc} .

As Fig. 1 shows, the FF for a bilayer organic solar cell can exceed the SQL. To find the possible reasons of high FF , we extended our model for bilayer organic solar cells to inorganic solar cells replacing heterojunction by homojunction and the field-dependent interfacial charge generation/recombination by bulk generation of free charges. As a result, the model gives the maximal FF according to the SQL. We discuss how interface charge generation/recombination and energy barriers in heterojunction could contribute to high FF in organic solar cells.

1. W. Shockley and H.J. Queisser, "Detailed Balance Limit of Efficiency of p-n Junction Solar Cells", *J. Appl. Phys.* **32**, 510 (1961).
2. M.A. Green, "General Solar Cell Curve Factors Including the Effects of Ideality Factor, Temperature and Series Resistance", *Solid-State Electronics* **20**, 265 (1977).
3. M.A. Green, "Solar Cell Fill Factors: General Graph and Empirical Expression", *Solid-State Electronics* **24**, 788 (1981).
4. C.W. Tang, "2-Layer Organic Photovoltaic Cell", *Appl. Phys. Lett.* **48**, 183 (1986).
5. M. Hirade, C.Adachi, "Small molecular organic photovoltaic cells with exciton blocking layer at anode interface for improved device performance", *Appl. Phys. Lett.* **99**, 153302, (2011).
6. V.A. Trukhanov, V.V. Bruevich and D.Yu. Paraschuk, "Effect of doping on performance of organic solar cells", *Phys. Rev. B* **84**, 205318 (2011).