Chapter 104
Organic Solar Cells Modeling and Simulation

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ABSTRACT

Modelling and simulation of organic (polymer, dye sensitized, and nanotube) solar cells is discussed. High J-V theoretical curves, the calculation of key parameters, and also the relative influence of different parameters on the cell operation, are evidenced and analyzed. On this basis, the authors obtain information on the optimization of the solar cell design and manufacturing.

MODELING AND SIMULATION OF ORGANIC CELLS BASED ON POLYMERS

Introduction

The polymer-based photovoltaic devices present some important advantages, such as the low cost and the easy manufacturing from thin films by chemical/physical vapour deposition, screen-printing, or casting. The band gap of the films can be adjusted by chemical synthesis to convenient values and the carrier mobility can reach 10 $cm^2/V{\cdot}s$ (Dimitrakopoulos & Mascaro, 2001; Kwok, 2003). Therefore, the polymer-based photovoltaic cells are competitive with those based on amorphous silicon, so that the interest for both the properties of the polymer materials and the characteristics of the polymer-based cells increases.

The first structure was a Schottky diode type structure, which has a conversion efficiency under 1%. In 1986, Tang (1986) introduced the planar donor-acceptor heterojunction, which has a higher conversion efficiency. Hiramoto, Fujiwara, and Yokoyama (1991) developed this idea. Tang introduced the concept of Bulk Heterojunction—BH. Xue et al. (2005) introduced the concept of Hybrid Heterojunction (HH) with higher efficiency 5%.

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Solar cells based on organic polymers used photoinduced transfer of electrons from semiconductor polymers, donor / acceptor polymers or acceptor molecules (such as C_{60}). Pairs of layers polymer / fullerene have a poor conversion efficiency of solar cell. Nanomorfological control at nanoscale of the separate regions in an interlaced network (BH) significantly increased the conversion efficiency of solar energy cells made of MDMO-PPV/C_{60}. Typical dimensions of the separate regions must be smaller than the exciton diffusion length. On the other hand, bicontinue percolation paths for the transport of charge carriers at the electrodes must be provided in order to increase the transport of charge carriers in organic and polymeric materials, and for mesoscopic order to improve crystallinity. So, an interlaced network at nanoscale with crystalline order of the both constituents is formed (these ones belong to individual sub-networks). Such a network is a convenient structure for the active layer of polymer PV devices. At the same time, forbidden bands of the photoactive layer materials should be chosen in order to absorb more light in solar radiation spectrum.

Using a mixture of MDMO-PPV soluble fullerene derivative (for example PCBM), it is possible to obtain solar cells with a 2.5% conversion efficiency.

It was shown (Shaheen, et al., 2001) that a conversion efficiency of 2.5% (for AM 1.5) can be obtained using chlorobenzenes as a solvent for the deposition by centrifuging in the mass ratio of 1:4 for the MDMO- PPV: PCBM. Using chlorobenzenes instead of toluene nanomorfology changes were remarked and the efficiency conversion increases 3 times. Such BH solar cells contain 80% PCBM. However, the MDMO-PPV polymer could be the main light absorber from these solar cells, because PCBM does not achieve almost no absorption in the visible and near infrared region. So an increase in volume concentration of MDMO-PPV was necessary for a better absorption of sunlight.

The electron mobility from pure PCBM is proved to be higher $(\sim 10^{-3}\ \mathrm{cm}^2/\mathrm{Vs})$ compared to the holes mobility from the MDMO-PPV $(\sim 10^{-4}\ \mathrm{cm}^2/\mathrm{Vs})$ and the holes mobility in the mixture increases with the increasing of fullerene mass, despite of the fact that the addition of fullerene introduces more defects (which would reduce the mobility).

By replacing in PCBM the C_{60} fullerene with C_{70} one, the HOMO-LUMO transition would be easier and would increase the absorption of light. An improved efficiency of BH solar cells in isomeric mixture of MDMO-PPV and C_{70} derivatives was obtained (Wienk, et al., 2003). Mixtures of this kind are suitable when they are prepared from a solution of o-dichlorobenzene (ODCB) and solar cells have a conversion efficiency of $\eta = 3\ \%$ for PM 1.5.

Operating Principle of Polymer-Based Solar Cell

The process of conversion of light into electricity using a organic solar cell (Figure 1) can be plotted by the following steps: 1) absorption of a photon determining the formation of an excited state, that is, the creation of an exciton (electron-hole pair); 2) exciton diffusion to a region where dissociation occurs; 3) charge transport within the organic semiconductor to the respective electrodes.

The obtained photo-voltage is a direct result of the departure from thermodynamic equilibrium state after the movement of charge carriers, generated by solar radiation under the action of local fields, which in the case of organic semiconductors is due to the change in chemical composition. Because of the large band gap in organic materials, only a small portion of the incident solar light is absorbed. A band gap of 1.1 eV (1100 nm) is able of absorbing 77% of the solar irradiation on Earth (Nunzi, 2002). But, the majority of semiconducting polymers have band gaps higher than 2 eV (620 nm), which limits the possible harvest-