

## Organic Solar Cell

### Introduction:

The aim of this assignment is to get you aware about the various materials/structures used in the fabrication of organic and in-organic solar cells and their repercussion/implication on the efficiency determining parameters i.e.  $J_{sc}$ ,  $V_{oc}$  and  $FF$ . But, before starting the analysis, you need to be familiar with properties of materials used and with their interfaces. It is assumed that you are familiar with  $I$ - $V$  characteristics of organic devices, MATLAB and have a little bit insight of fabrication process of organic devices.

### Theoretical section:

1. What is the major difference in working principle of in-organic and organic solar cells? What is the highest reported efficiency for single junction structures in both cases? What is the main reason behind such a large difference?

2. An excerpt is taken from a paper *"It's found after analyses that in in-organic solar cell (Si),  $V_{oc}$  is limited by built-in voltage (0.7 V) of the junction i.e. material dependence, while in case of organic solar cell,  $V_{oc}$  is found to be a function of difference of work functions of electrodes i.e. contact dependent."* Justify the above statement and comment on validity of above argument.

3. A new organic material is brought from a manufacturer and the quoted value for its band gap is 2.1eV. What other tests one must perform on material before going for fabrication of standard bi-layer solar cell with ITO anode and  $C_{60}$  as acceptor?

4. The standard structure of Bulk heterojunction devices is ITO coated glass- active layer-metal cathode. So, the inverted structure would be Glass substrate-metal cathode-active layer-ITO coated glass. For the time being, assume both structures can be made with equal ease. Which one is likely to give better efficiency under light? Why is the first structure generally preferred over second?

5. Five sets of devices (solar cells) are made simultaneously (batch processing) with following layer structures:

- (1) ITO: polymer1: metal
- (2) ITO: polymer2: metal
- (3) ITO: PCBM: metal
- (4) ITO: (blend of polymer1 & PCBM): metal
- (5) ITO: (blend of polymer2 & PCBM): metal

Assume both polymer1 & polymer2 has energy levels similar to P3HT and

(i) Mobility of holes in polymer1 is equal to mobility of electrons in PCBM

(ii) Mobility of holes in polymer2 is two orders of magnitude greater than that of electrons in PCBM and the HOMO of polymers are aligned to work function of ITO and LUMO of PCBM is aligned to work function of metal cathode i.e. in bulk, contacts are ohmic.

\*Polymers are considered to be hole conducting and PCBM as electron conducting material.

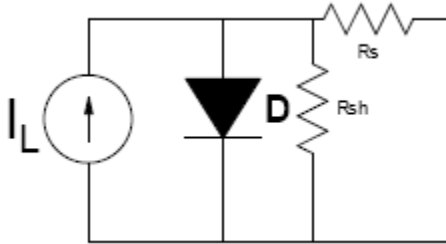
Draw the approximate  $I$   $V$  characteristics for all 5 devices under (dark & light) for voltage swing of -5V to 5V.

**Simulation Section:**

Power conversion efficiency of the solar cell is given by  $\eta = (V_{oc} * J_{sc} * FF) * 100 / P_{in} \%$

Where,  $FF$  = fill factor,  $V_{oc}$  = open circuit voltage,  $J_{sc}$  = short circuit current,  $P_{in}$  = incident power.

The equivalent circuit model for solar cell is



Where,  $I_L$  is the number of dissociated excitons per second.

$D$  represents dark I V characteristics of solar cell

$R_{sh}$  represent shunt resistance,

$$R_{sh} = \left[ \frac{dI}{dV} \right]_{V=0}^{-1}$$

$R_s$  represent series resistance,

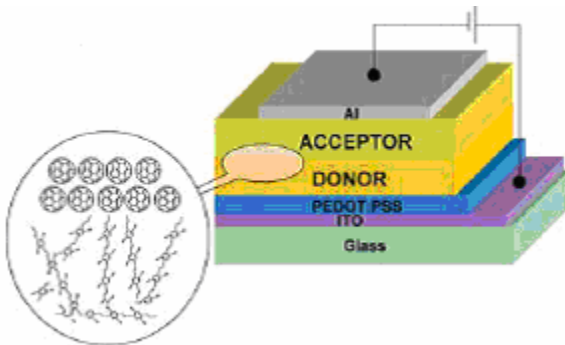
$$R_s = \left[ \frac{dI}{dV} \right]_{I=0}^{-1}$$

**Part A: Parameters extraction**

Given the J V characteristics in 4<sup>th</sup> quadrant, write a MATLAB code that extract out  $V_{oc}$ ,  $J_{sc}$ ,  $FF$ ,  $\eta$ ,  $R_{sh}$  and  $R_s$  from the input J V characteristics.

**Part B: Calculation of  $\eta$  (efficiency)**

The simplest efficient organic solar device is a bi-single layer structure donor and acceptor sandwiched between two electrodes.



Calculations for  $\eta$ 's are done by first calculating  $J_{sc}$  from  $\eta_{IQE}$  (internal quantum efficiency),

$$\eta_{IQE} = \eta_A \eta_{ED} \eta_{CT} \eta_{CC}$$

For, an absorbing organic layer of donor thickness  $d$ , we have

$$\eta_A = (1 - e^{-\alpha d})$$

$\alpha$  = absorption co-efficient as function of wavelength.

$$\eta_{ED} = e^{-d/L_d}$$

$L_d$  = diffusion length

$$\eta_{CT} = (1 - Q1)$$

$Q1$  = Quenching fraction at dissociation site

$$\eta_{CC} = e^{-t/\zeta}$$

$\zeta$  = recombination life time

All above parameters are used in final calculation of short circuit current.

$\eta_{\text{QE}}$  is basically a ratio of total number of electrons/holes collected at electrodes to incident number of photons. Total number of (electrons/holes) collected per second defines the current.

**Step 1: Calculation of  $\eta_{\text{A}}$**

Starting point will be to calculate total number incident photons per second for each wavelength absorb by the material ( $\eta_{\text{A}}$ ). Assuming exponential profile of light inside donor ( neglecting optical interferences) and taking effective thickness of solar cell for light absorption as thickness of donor material (approximation).

Calculate the total number of photons absorbed inside donor by integrating sun spectrum with absorption spectrum of material. (Both spectrums are given in appendix).

**Step 2: Calculation of  $\eta_{\text{ED}}$**

Exciton diffusion efficiency is obtained by convolution of exciton profile over a distance  $d_1$  (donor length) using diffusion coefficient  $L_d$ .

Then, integrating for all wavelengths, you will have all excitons per second reaching the donor-acceptor interface.

**Step 3: Calculation of  $\eta_{\text{CT}}$**

Assuming any reasonable quenching fraction, calculate number of carriers ready to go towards electrode.

**Step 4: Calculation of  $\eta_{\text{CC}}$**

Assuming electron mobility is lesser than hole mobility, calculate the time take by electron in reaching cathode and incorporate recombination life time in calculating total number carriers reaching per second at cathode. Multiply the total number of carries with a charge of electron results total charge reaching cathode per second, i.e., current. Consider it as short circuit current.

**Step 5: Calculation of  $\eta$**

Assume any reasonable value of FF and take  $V_{\text{oc}}$  as difference of electrode work functions. Multiply all to get efficiency  $\eta$ . Take anode workfunction as 5.1eV.