Interface roughness in OPV device

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The performance of OPV (Organic photo voltaic) or OSC's (Organic solar cell) devices are depend on mobality of free electron and holes generated in organic active layer. The interface between donar and acceptor layer are active site for exciton dissociation. The number of free electron and holes formed after dissociation of exciton are major contributor of Jsc. We also study the effect of roughness of Phthalocyanine (small molecule organic material) as donar layer with C_{60} as acceptor layer in bilayer OPV device. We have studied the AFM and XRD of copper phthalocyanine (CuPc), zinc phthalocyanine (ZnPc) and Metal free phthalocyanine (Hydrogen Phthalocyanine - H_2Pc). We found that the selections of active layer material in OPV device are such that the roughness level of both materials forms maximum interface area between donar and acceptor.

Keywords: Phthalocyanine, AFM, Interface roughness.

1. INTRODUCTION

OPV devices are the most promising alternative source of energy as they can play an important role in generating clean and cheap energy [1]. A typical OPV device contains the organic semi conducting material sandwich between two electrodes named as anode and cathode. This potential of OPV devices has been recognized and elaborated research is being done all over the world to improve performance. Various physical treatments, new device designs and the advanced materials have been employed to enhance the performance of OPV device. The donor-acceptor concept was the most important finding for efficient OPV devices. In the donor-acceptor hetro-junction approach the photo-generated excitons could easily be dissociated into free carriers at the donar-acceptor interface [2,3,4]. Free holes and electrons are transferred to the respective electrodes and collected there.

The performance of an OSC is determined by measuring the current density-voltage (*J-V*) characteristics under sun light illumination. A photovoltaic device under illumination is characterized by open circuit voltage (V_{oc}), short circuit current density (J_{sc}), fill factor (*FF*) and power conversion efficiency (PCE). *FF* is the ratio of the maximum power output (P_{max}) of the cell over the product of J_{sc} and V_{oc}. Current and voltage corresponding to P_{max} are represented as J_{max} and V_{max}. A typical *J-V* characteristic of a solar cell is illustrated in Figure 1. The points corresponding to J_{sc}, V_{oc}, J_{max} and V_{max} are clearly shown in the figure.

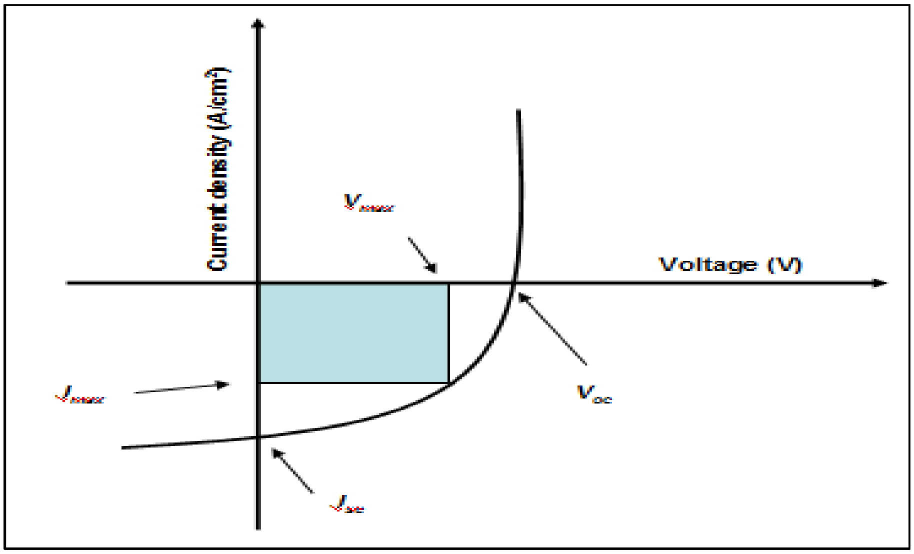


Fig. 1: Typical *J-V* characteristics of a solar cell, the shadowed area indicates the maximum power that can be extracted.

V_{oc} of a solar cell is defined as the voltage developed between the two electrodes of the illuminated cell when there is no external load. J_{sc} of a solar cell is defined as the current in the external circuit when the external load is short circuited. On the *J-V* curve it is the photo-generated current by the device when there is no applied voltage. Photo-generated current is directly related to optical and electrical material properties. *FF* is a fraction of ideally maximum achievable power of the device under illumination or is defined as the ratio of maximum power actually achieved (P_{max}) over the ideally maximum achievable power ($J_{sc}*V_{oc}$) i.e.

$$FF = \frac{J_{\max} * V_{\max}}{J_{sc} * V_{oc}} = \frac{P_{\max}}{J_{sc} * V_{oc}} \tag{1}$$

P_{max} indicates the maximum power that can be extracted from the solar cell and it is represented as the area of the filled rectangle in Fig.1. Efficiency of solar cells is the most important parameter as it indicates how efficiently the cell operates, and it is defined as the electrical power output over the incident optical power. It can be calculated from

$$PCE(\eta) = \frac{J_{sc} * V_{oc} * FF}{P_{in}} \tag{2}$$

where P_{in} the incident solar radiation in W m^{-2}.

The shape of *I-V* curve is a measure of the *FF* i.e. concave shapes give higher *FF* values whereas convex shapes gives lower *FF* values. In general, large series resistance, small shunt resistance and recombination tend to reduce *FF*. The values of Current flow in material are depend on the morphology of the material and the interface between donar and acceptor layer. For study the roughness of Donar material we study the AFM images.

2. ATOMIC FORCE MICROSCOPE (AFM)

In all Scanning Probe Microscopes (SPM) techniques a tip interacts with the sample surface through a physical phenomenon. Measuring a “local” physical quantity related with the interaction, allows constructing an image of the studied surface. All the data are transferred to a PC, where, with the use of the appropriate software, an image of the surface is created. The AFM measures the forces acting between a fine tip and the sample. The tip is attached to the free end of a cantilever and is brought very close to a surface. Attractive or repulsive forces resulting from interactions between the tip and the surface will cause a positive or negative bending of the cantilever. The bending is detected by means of a laser beam, which is reflected from the back side of the cantilever. Fig.2 shows the basic concept behind operation of an AFM.

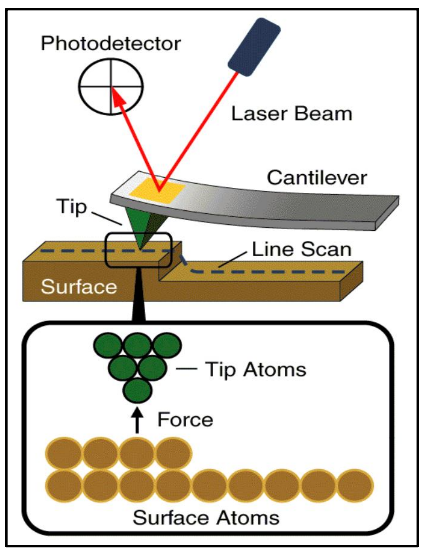


Fig. 2: Basic concept behind operation of AFM.

AFM is currently applied to various environments (air, liquid, vacuum) and types of materials such as metal semiconductors, soft biological samples, conductive and non-conductive materials. With this technique size measurements or even manipulations of nano-objects may be performed. A force sensor in an AFM can only work if the probe interacts with the force field associated with a surface [5].

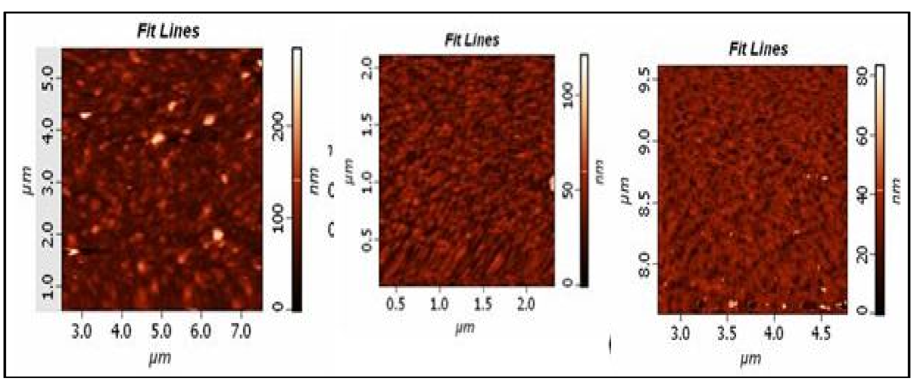
3. EXPERIMENT

For determination of roughness we prepared thin film of CuPc, H_2Pc and ZnPc on glass surface via thermal evaporation technique. The evaporation rate of the source material was controlled by this current. An oscillating quartz crystal thickness monitor DTM-101 from Hind Hi Vacuum, Bangalore, was used to determine the thickness of the film deposited on the substrate. The speed of coating or evaporation is maintained to 4~6 Å /s under the vacuum of 10^{-6} mbar.

4. RESULT AND DISCUSSION

In OSCs roughness of donor layer plays important role, it provides interface for effective exciton dissociation into free electrons and holes. This is the primary requirement to get maximum interface between donor/acceptor layers, and bulk hetrojunction OSCs have good advantage over bi-layer OSCs. For batter performance of device it should be optimize as large roughness also retards the efficiency of solar cell via reduction in contact between donor and acceptor. Veeco (USA), AFM was used for the surface roughness studies of the materials.

The nitrogen-metal distance in platinum phthalocyanine is 2.01 Å as compared with 1.92 Å and 1.83 Å in the metal-free and the nickel compound respectively [6]. In 1936, it was already known that 4-coordinate bivalent copper can exhibit planar symmetry. This behaviour is not same with other phthalocyanines except the magnesium derivative [7]. X-ray evidence and deductions therefrom by Robertson in 1935 established that the central metal atom copper and the four surrounding isoindole nitrogen atoms are coplanar [8]. The diameters of atoms in crystals of copper are 2.6 Å [9]. These dimensions emphasize the “close fit” of these atoms in the central open portion of the phthalocyanine molecule. Fig.3. shows the 2D and 3D AFM images of CuPc, H_2Pc and ZnPc thin films. Roughness for a 5x5 μm^2 CuPc sample was found to be 17.6 nm.



(a) CuPc (b) H_2Pc (c) ZnPc

Fig. 3: 2D AFM image thermal evaporated CuPc, $H_2Pc$and ZnPc thin film.

Roughness of 2x2 μm^2 H_2Pc sample is found to be 7.9 nm and Roughness of 2x2 μm^2 ZnPc sample was found to be 4.58 nm (see Table 1). The roughness in Pc’s are found to be in the order of CuPc > H_2Pc > ZnPc. When we correlate it with the performance of OSC's manufactured in different configurations. We found that the efficiency of OSC's based on respective Pc's gives the Short circuit current density in the sequence of ZnPc > H_2Pc > CuPc based solar cell.

Table 1: Roughness of Different MPc's.

S.No.	Material	Sample size	Roughness
1	CuPc	5X5 μm^2	17.6 nm
2	H_2Pc	2X2 μm^2	7.9 nm
3	ZnPc	2X2 μm^2	4.58 nm

We assume that the reason behind the variation in performance of OSC's is in case of CuPc interface with C_{60} the higher roughness of Donor film may restrict the contact interface area with C_{60}, which is dissociation site for excitons.

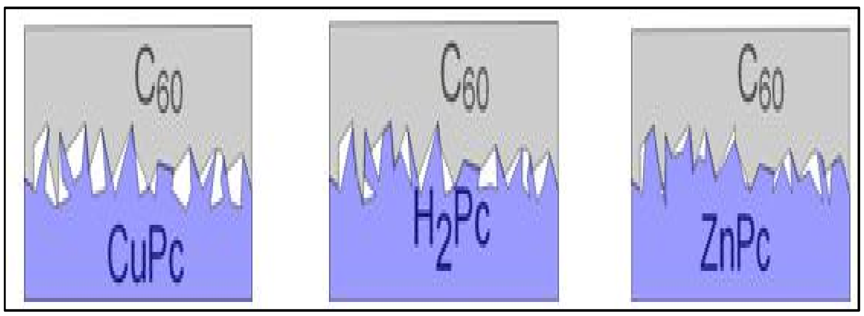


Fig. 4: Schematic diagram to illustrate the contact interface between Pc's with C_{60}.

As the roughness reduces from H_2Pc to ZnPc the contact interface increases and more excitons can be dissociated into free electron and hole and overall short circuit density is found to increased (see Figure 4). The lower value of current in CuPc is due to the lower interface area between donar and acceptor layer. In our The order of *Jsc* found to be ZnPc < H_2Pc < CuPc based OPV devices. Increase the contact area at organic/cathode interface for effective exciton dissociation and to restrict the exciton quenching at organic/cathode interface is a noble idea by which we can utilise the maximum excitons for maximum generation of free electrons and holes.

5. CONCLUSION

By AFM images of CuPc and ZnPc layers shows that the roughness of CuPc is higher than ZnPc when they are coated by thermal evaporation technique in identical processing conditions. These properties of ZnPc, CuPc and H_2Pc are basic fundamental properties which are responsible for different comparative performances in photovoltaic devices based on these phthalocyanines. Mismatch of roughness of Donar and acceptore is very important parameter for efficient solar cells. AFM studies give the idea of interface formed between donor and acceptor materials. The roughness difference between donor and acceptor must be minimum as in case of ZnPc/C_{60} this roughness difference is lower than $CuPc/C_{60}$ and results says that $ZnPc/C_{60}$ based OSC has higher short circuit density than that based on $CuPc/C_{60}$. Enhancement in interface area and interface layer at the donor/acceptor interface with controlled nano-scale islands which participated in the enhancement of V_{oc} and J_{sc} in a controlled fashion also improved the performance [10].

6. ACKNOWLEDGMENT

I did this experimental work at NPL New Delhi, when I was doing my Ph.D. I would like to pay my heartfelt gratitude to my supervisor Dr. S. Chand for their kind help and support. I heartily thank him for providing me the facilities and a healthy working environment at NPL.

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