

Characterization of Bi Layer Organic Solar Cell Using Silvaco TCAD

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Abstract - Organic solar cells have gained serious attention during the last few years and are becoming established as one of the future photovoltaic technologies for low-cost power production. During last 10 years lot of work has been done on this technology. Some of them are polymer fullerene solar cells, small molecule and hybrid solar cells. The most successful of them are the polymer–fullerene solar cells that comprise a mixture of the polymer, which is the donor material and a fullerene material as the acceptor material. While research on organic solar cells date back to the 1980s the first example of a polymer solar cell was the bi-layer hetero junction between the soluble polymer and the Buckminsterfullerene C60 where a power conversion efficiency of 0.04% was obtained using monochromatic light. The next convincing step was the application of a dispersed bulk hetero-junction of MEHPPV and C60 and later soluble derivatives of C60 which increased the power conversion efficiency to 2.5%. The third step is The most important physical means for improving performance are the use of a thin layer of an insulator between the active layer and the low work function metal electrode and more recently also in inverted devices, the use of optical spacers, the understanding of how the open circuit voltage is obtained and by these means deriving an efficient method for predicting performance of materials combinations based on measurable materials properties.

Key Words: Organic solar cells, work function, efficiency, the bilayer hetero junction, exciton

1.INTRODUCTION

Organic and inorganic materials are two different types of materials. In organic solar cells whenever the electrical transport is studied, all the properties of semiconductor such as, mechanical, electrical, optical and chemical should be always keep in mind. At this point we study about these properties and relations between them, which describe some concepts like exciton, Fermi level and etc. Now we present a small part of metal-semiconductor junction theory and in any type of electrical device it is very convenient for the study of electrode interfaces. By the detection of good semiconductor properties as well as technological properties for example flexibility and low cost confession, investigators became greatly encouraged and motivated. Deep-rooted theories of solid state physics together with the band theory provide many concepts such as valence band and conduction band. To explain the physics of electronic devices these concepts are very beneficial. Concepts like localized and

delocalized have been accustomed model their muddled nature and their great amount of traps for the amorphous type inorganic materials. By localized states the way of charge transport becomes conquered in amorphous materials. Small molecules materials and polymer materials are two types of organic semiconductor materials. The solicitations of the concepts conferred above to organic materials depend on the variety of used organic semiconductor in it. Occasionally crystalline models have been used to study crystalline structures for the reason that small molecule type organic semiconductor materials have crystalline structures.

The physics behind hand the polymer materials are much closer to the amorphous inorganic material than crystalline ones. It is just as a result of the amorphous nature of polymer material. Nevertheless, one property is communal to all organic semiconductors i.e. the occurrence of localized states whose beginning their band nature. Electrical models do not contemplate such localized states so that it appears unfeasible the use of these electrical models.

For the study of the solar cells we can excellently applies recent models together with organic materials. Those models which frequently consider localized states but occasionally interface states, we primarily recommended for inorganic semiconductors and then corresponding models can be applied to the organic semiconductors.

1.1 Types of organic semiconductors and their structural properties

Organic materials frequently comprise carbon. Formation of hexagonal and pentagonal molecules is the core of maximum organic semiconductors.

This creation of molecules is leaded by the propensity of carbon component which bond to other carbon atoms. To form organic semiconductors, small molecules bind other small molecules chemically and these small molecules are identified as monomers. According to their chemical structures these materials are separated into two general types i.e. oligomers and polymers. Oligomers are mostly completed by only limited monomers and are molecules. Polymers are also formed by monomers but the difference in establishment of polymers and oligomers is that in oligomers we need only few monomers but in polymers we need more than 10 monomers.

Systems of molecules which are created by oligomers and polymers is allied by Van der Waals forces. Systems of molecules are known as macromolecules having some macroscopic structural properties which are usually depend on their method of deposit and chemical structure. Sublimation temperatures of smaller molecules are inferior and naturally these molecules are more soluble. On the other hand enhanced films upon spin coating are just provided by large molecules. Thermal evaporation technique is used for the deposition of oligomers while we use wetting processes for the better deposition of polymers. High vacuum circumstances and high temperatures are requisite for the establishments of devices through thermal sublimation while wetting processes can be implemented at room temperatures and ambient pressures. Chromophores are referred to as dyes if they are evidently soluble. But firstly, we should know about chromophores. It is as when visible light are frequently absorbed by oligomers and monomers, these oligomers and monomers are recognized as chromophores. If chromophores are not evidently soluble then chromophores are referred as pigments.

The concepts of dyes and pigments can be certainly comprehended by the figure (a). The type of material can be describe by the variation in chemical structures means if there is any type of adjustment in chemical structure of material then we will know that which type of material is used.

2. Organic Solar Cell Technology

The alteration of single and double bond i.e. σ and Π bond make to organic semiconducting materials make novel. This alteration make conjugated organic materials to partially covalent as well as partially polar. So materials having such property show novel bond characteristic. This type of materials show large electron lattice coupling as compare with traditional semiconducting materials, and this electron lattice coupling result in that most of charge to be localized. So there is need of additional energy to generate charge carrier.

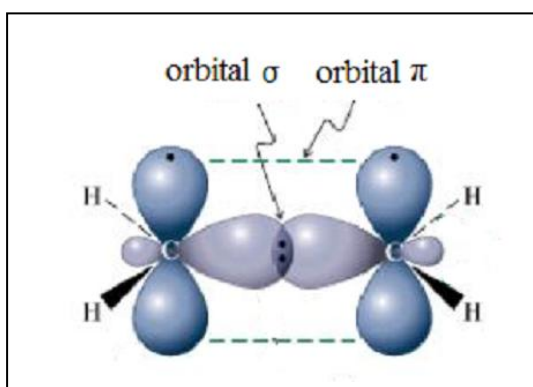


Fig -1: Sigma and Π bonding in ethane compound

Every molecules in above figure is structured by sp^2 hybridization of atom, in sp^2 hybridization the electron of Π orbital is loose from the carbon core so the polarization of these Π electron is easy and they become charge carrier. The fully-filled orbital made by Π bond electrons is known as HOMO and the empty orbital's having high energy level is known as LUMO. Figure shows the position of highest occupied molecular orbital and lowest unoccupied molecular orbital.

Organic photovoltaic materials can be of two types: one is polymers and other one is small molecule organic materials. There is large difference in the property of these two. Polymers are made by an arrangement of the chain of basic units. Polymers can be used in liquid form. On other hand the molecules organic materials are the compositions of small molecules.

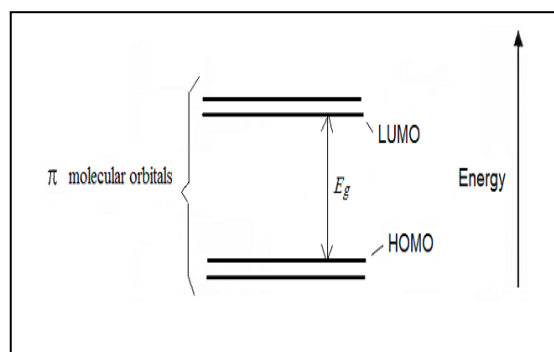


Fig -2: Scheme of HOMO AND LUMO orbitals

3. Design and implementation of Bi-Layer Organic solar cell

In a bilayer hetero-junction device, p-type and n-type semiconductors are sequentially stacked on top of each other. Such bilayer devices using organic semiconductors were realized for many different material combinations. In such devices, only excitons created within the distance of 10-20 nm from the interface can reach the hetero-junction interface. This leads to the loss of absorbed photons further away from the interface and results in low quantum efficiencies [45]. The efficiency of bilayer solar cells is limited by the charge generation, 10-20 nm around the donor-acceptor interface (Figure 4.1). Using thicker films creates optical filter effects of the absorbing material before the light gets to the interface, resulting in a minimum photocurrent at the maximum of the optical absorption spectrum [46]. Also, the film thicknesses have to be optimized for the interference effects in the multiple stacked thin film structure [47, 48].

Bi-layer organic photovoltaic is a single junction organic cell in which two material form junction. One material is donor and other is acceptor. MDMO-PPV (Poly[2-methoxy-5-(3',7'-dimethyl-octyloxy)-p-phenylenevinylene]), PFB (poly(9,9

diocetylfluorene-co-bis-N,NO-(4-butylphenyl)-bis-,Nophenyl-1,4-phenyldiamine)), P3HT(Poly-3-hexylthiophene), MEH-PPV, PPV are the donor materials and CN-MEH-PPV(poly(2-methoxy-5-5ethylhexyloxy-1,4-phenylenecyanovinylene)), PCBM, F8BT poly(9,9-dioctylfluorene-cobenzothiadiazole), C60, PC60BM, C70BM, P61BM are the acceptor materials. This work has been done by taking many of above materials as acceptors and donor and selected best one that give height efficiency.

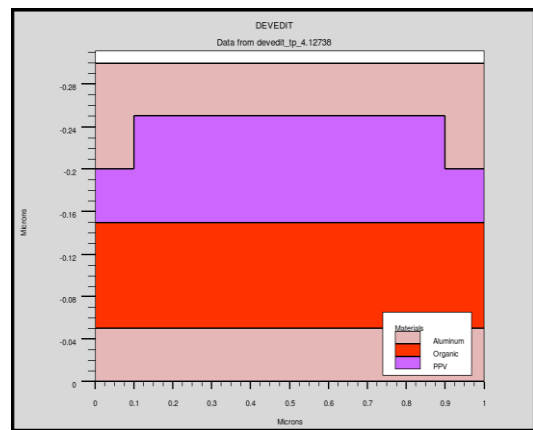


Figure 4.2 Device structure of Bi-Layer solar cell with inserted Electrode

Variation in Efficiency with Different Materials

Table-1: Materials property for different materials

Materials Used	Permittivity ($\times 10^{-11}$)	Electron Affinity (eV)	Band gap (eV)	Electron Mobility (10^{-6})	Hole Mobility (10^{-6})
ZnPc	2.86	5.28	2.69	8.7	8.56
MEH-PPV	3.0	2.8	2.1	5.6	5.34
ZnPc(Pure)	2.8	5.20	1.97	1	.96

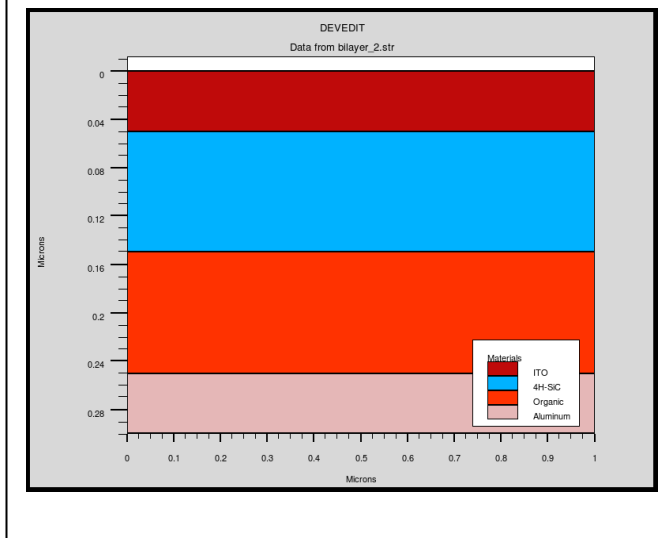
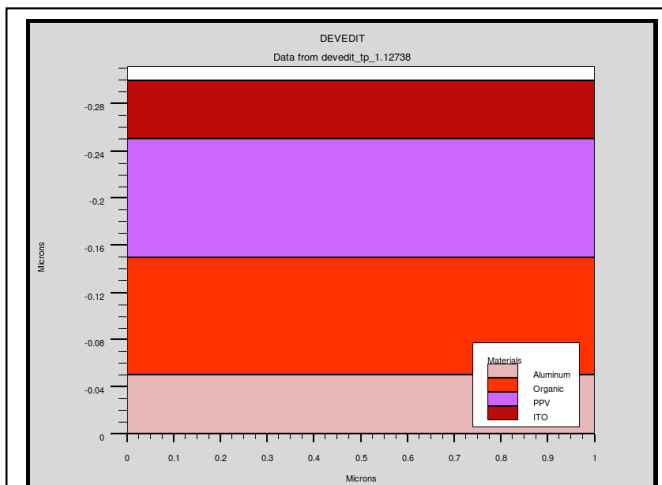


Figure 4.1 Device structure of Bi-Layer solar cell

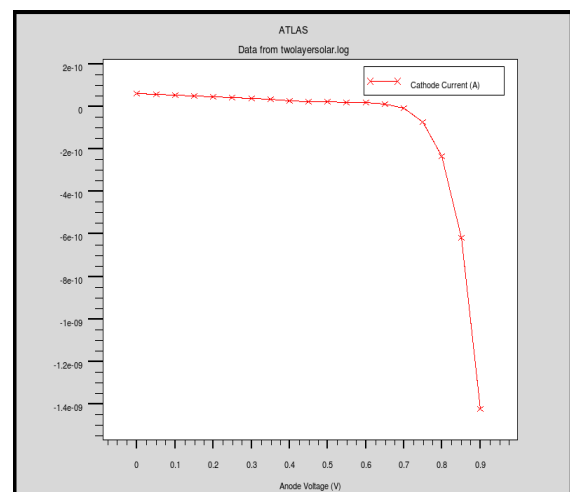
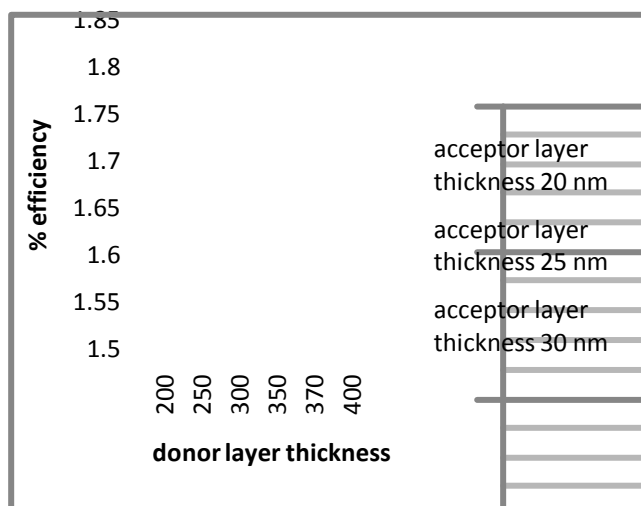


Chart -1: Anode voltage Vs cathode current with inserted electrode

Efficiency variation with change in donor layer Thickness

As the mobility of an organic photovoltaic is very less as compare with Si crystal so the device structure is an important factor which effect to the efficiency of OPV, further increases in efficiency have been limited by low electron mobility. Optimizing the efficiency of polymer-based, planar organic solar cells requires nano scale control of the thicknesses of constituent layer materials composing the device. A thin film optical simulation modeling tool has been used to determine ideal active layer thicknesses for region regular poly (3-hexylthiophene) and phenyl-C61/C71-butyrac acid methyl ester (P3HTPC61BM) organic blends used as photoactive components in polymer solar cells. As shown in table 4.4 and table 4.5 when its start from the lowest thickness the efficiency of organic photovoltaic increase i.e. as the number of mobile carrier increase with increase in the thickness of materials.



3. CONCLUSIONS

Many solar cell technologies exist for the direct conversion of light into electricity, each with its own advantages and disadvantages. One of the most important metrics for determining the competitiveness of different solar cell technologies is the expected cost per watt produced. There are many strategies being pursued to achieve cost efficiency such as improving efficiency of standard silicon cells, reducing the amount of expensive raw materials with thin films, developing low cost manufacturing methods, and designing high-efficiency devices with small areas. Organic solar cells are a newer technology in this field and have the potential for low manufacturing and material costs. Many challenges still remain for moving organic solar cells from the laboratory into high-volume commercial applications. In particular, some of the needs in organics are a clearer understanding of the device physics, refinement of high-volume fabrication techniques, improvements in overall

power conversion efficiency, development of large area devices, flexible encapsulation, and evaluation and, most likely, improvement of stability under operation. This thesis looked at organic solar cells based on bi-layer hetero-junctions and bulk hetero-junction as model systems to review many of the current theories regarding electrical processes in the devices and to expand on what mechanisms could be responsible for the open-circuit voltage and reverse saturation current.

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