Device Fabrication and Optimisation of P3HT:PCBM based Organic Photovoltaics

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Abstract

The maximum efficiency for the prominent material system in OPVs, namely the mixture of poly(3-hexylthiophene):[6,6]phenyl-C61butyricacidmethylester(P3HT:PCBM) is calculated to be 33%. But in practical maximum reported efficiency is 6%. This is because of four types of loses; optical, exciton, recombination and collection loses. Hence it's essential to optimize the device fabrication conditions. This work attempts the fabrication and analysis of I-V curve obtained for the mentioned combination. Various parameters like mixing ratio, temperature, pressure, inert atmosphere, vacuum condition, spin coating speed, thickness and compounds used for intermediate layers were varied and the cell was optimized for maximum photocurrent and best power conversion efficiency

The basic structure of an organic solar cell is formed by contacting semiconducting electron donor and acceptor compounds (p/n type). Interpenetrated networks of the donor and acceptor materials came as an improvement in the structure, known as bulk heterojunction (BHJ) solar cell. They had very high power conversion efficiencies due to the dramatic increasing of the contact area between the D/A materials leading to a significant increase of the number of generated excitons as well as their dissociation into free charge carriers. The basic optical and electronic processes in BHJ solar cells can be summarized in 4 steps

- (i) Formation of the exciton by the optical absorption of sunlight
- (ii) Migration of exciton to the donor- acceptor interface
- (iii) Formation of electron and holes by exciton dissociation
- (iv) Transportation and collection of charges at the electrodes.



In BHJ OPV excitons whose dissociation into free carriers is not straightforward. Due to the low dielectric constants of organic compounds, it needs to reach the donor-acceptor interface to dissociate into free charges; the driving force for this exciton dissociation being provided by the energy difference between the molecular orbitals of the donor and acceptor. The transport of the thus generated free charges toward the electrodes represents another important issue. Another problem is that organic materials have charge carrier mobility significantly lower than those of inorganic semiconductors, because charge carrier mobility is strongly dependent on the molecular organization of the material. In order to achieve better efficiencies,

a good control on the morphology of the donor-acceptor materials at a nanometre scale is necessary. Furthermore,

it's also essential to prevent charge recombination (geminal or bimolecular) processes which result in lower energy conversion efficiencies. In summary, an appropriate choice of the donor and acceptor materials is critical to ensure a good match between them in terms of optical, electronic and morphological properties, which eventually determine the effective photocurrent and performance of the PV device. Therefore, the rational design of new materials able to improve some specific demands within the PV device is critical for the successful development of competitive solar cells.

ITO substrates of 3 x 3 dimensions were taken cleaned with soap water followed by deionized water. Substrates were etched using zinc powder and hydrochloric acid. Etched substrates were cleaned with soap water and were ultrasonicated for 15 minutes with deionized water followed by acetone and isopropanol. Dried substrates were UV-Ozonized for 40 minutes to increase the glass wettability. They were spincoated with (PEDOT:PSS) poly(3,4-ethylenedioxythiophene)-poly(styrene-sulfonate). This is added between the active layer and ITO because this buffer material helps to avoid local shunts, smoothing the ITO surface, enhancing adhesion to the upper light absorbing layer, providing better energy level matching, and improving device stability by hindering oxygen and indium diffusion into the active layer. At optimized rpm of 2800 for 60 seconds. Spincoated substrates were annealed at 120°C for 30 minutes. Annealed substrates were kept in vacuum for slow drying and were subsequently spincoated with 0.1mL P3HT: PCBM solution (15mg/mL concentration, kept stirred for 14h at 40°C) at different rpms. Active layer spincoated substrates were taken immediately for thermal evaporation. Aluminium layer of about 90nm thickness was deposited. The prepared solar cells were kept in vacuum and was then I-V characterized. From the I-V graph photocurrent was measured. Experiment was repeated with different masks hence changing the cell dimensions. Cells were optimized also by annealing at different temperatures after active layer spincoating.

Optimized thickness of about 100nm was obtained at 1000rpm spincoating for 60 seconds. Thoroughly stirred P3HT: PCBM mixture was used as the active layer in all the

solarcells prepared. When spincoted on top of PEDOT: PSS layer P3HT self-organizes into a microcrystalline structure and, because of efficient inter-chain transport of charge carriers, the (hole) mobility in P3HT is high (up to 0.1 cm²)

 V^{-1} s⁻¹). Moreover, in thin films interchain interactions cause a red shift of the optical absorption of P3HT, which provides an improved overlap with the solar emission.



The second component, PCBM, is a C60 fullerene derivative with an electron mobility of 2×10^{-3} cm² V⁻¹ s⁻¹ Compared to C60, the solubility of PCBM in organic solvents is greatly improved, which allows the utilization of film deposition techniques requiring highly concentrated solution. Also PCBM can crystallize and control nucleation and crystallization kinetics, allowing the adjustment of the crystal size. However, continuous crystallization may result in single crystals with micrometer sizes. Interestingly, the efficiency of solar cells based on P3HT and fullerenes was shown to depend strongly on the processing conditions and to improve particularly by a thermal annealing step.

The cell dimensions tested were 0.1 x 0.1, 0.2 x 0.2 and 0.6 x 0.6 (in cm). Cells of 0.6 x 0.6 dimensions gave best results during I-V characterization. The working of the cells depends of many parameters of processing. Proper ultrasonication followed by nitrogen flow treatment is very important for the cell to work properly. UV-Ozone treatment for 40 minutes was good for better performance. Presence of PEDOT: PSS layer is most beneficial for higher efficiency of P3HT: PCBM blend based solarcells. The PEDOT:PSS solution used should be at room temperature atleast for 30 minutes before spincoating. Also solution that had long shelf life is also not suitable for spincoating. The layer can facilitate efficient exciton dissociation and hole transport. Annealing of PEDOT: PSS layer after spincoating at 120°c for 30 minutes is crucial to get a uniform active layer. Concentration of the P3HT: PCBM solution need to be optimum to get uniform layer of desired thickness. 15-20 mg/mL concentration was found to give best results during spincoating. If the concentration is too low then only very few charge carriers will be generated and we can get only feeble photocurrent. If the concentration is too high thicker active layer will be formed and will result lesser mobility of charge carriers and higher risk of them being trapped in the active layer. During spincoating the blend solution when added on static condition rather than while rotation generated better films. Annealing of active layer at 110°c, 120°c and 180°c as studied. 10 minutes annealing at 120°c had good performance. Humidity conditions while processing seemed to affect the efficiency of cell significantly. So vacuum storage and inert atmosphere is necessary while device

fabrication. Another factor that influenced the cell performance was the chances of aluminium getting oxidized to alumina after thermal evaporation and thus preventing charge carrier flow. Atmost care should be taken to minimize the chances of such oxidation. From the I-V graph cells gave an open voltage around 1.5V. The current obtained was about 0.1 mA only. But in reverse bias there was a significant current generated in all the cases.



Solution made in 1:0.8 P3HT: PCBM ratio gave best performance. Processing in inert atmosphere is crucial for a high performing solar cell.The smaller photocurrent obtained might be due to the oxidation of thermally evaporated aluminium to alumina affecting charge transport. So thermal evaporation in nitrogen or argon atmosphere is suggested. The significant current obtained in reverse bias indicates defective charge transfer. Use of an interfacial film for good electron transport could be tried to enhance charge transfer. The humidity, temperature conditions also influences the performance of solar cell.

References

- 1. N. Armaroli and V. Balzani, Angew. Chem., Int. Ed., 2007, 46, 52
- D. Guldi and L. Echegoyen, Carbon Nanostructures web themed issue Organic photovoltaics : a chemical approach doi: 10.1039/c003088k
- D. M. Chapin, C. S. Fuller and G. L. Pearson, J. Appl. Chem., 1954, 25, 676.
- 4. G. Dennler, M. C. Scharber and Ch. J. Brabec, Adv. Mater., 2009, 21, 1323
- B. Kippelen and J.-J. Bre' das, Energy Environ. Sci., 2009, 2, 251
- B. C. Thompson and J. M. J. Fre' chet, Angew. Chem., Int. Ed., 2008, 47, 58; (d) S. Gunes, H. Neugebauer and N. S. Sariciftci, Chem. Rev., 2007, 107, 1324
- A. Hirsch, The Chemistry of Fullerenes, ed, Wiley-VCH, Weinheim, Germany, 2005
- D. M. Guldi and N. Martı'n, Fullerenes: From Synthesis to Optoelectronic Properties, ed. Kluwer Academic Publishers, Dordrecht, The Netherlands, 2002
- R. Taylor, Lecture Notes on Fullerene Chemistry A Handbook for Chemists, ed. Imperial College Press, London, 1999
- 10. F. Langa and J.-F. Nierengarten, Fullerene: Principles and Applications, ed,RSC, Cambridge, UK, 2007