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Taguchi optimization of device parameters for fullerene and Poly (3-octylthiophene) based heterojunction photovoltaic devices

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Abstract

Photovoltaic devices were fabricated with the structure ITO/fullerene/Poly (3-octylthiophene)/Au and device parameters were optimized using Taguchi optimization technique. Optimized parameter such as fullerene and Poly (3-octylthiophene) film thickness, annealing temperature and annealing duration are found to be as 110 nm, 45 nm, 120° C and 15 min respectively. Fabricated device with optimized parameters shows short circuit current density (J_{sc}), open circuit voltage (V_{oc}) and fill factor (FF) as 2×10^{-4} mA/cm^2, 0.47 V and 0.25 respectively. Effect of solvent casting on C_{60} layer was studied which shows formation of uneven surface providing large interfacial area.

Keywords: Fullerene; Poly (3-octylthiophene); Taguchi optimization; Photovoltaic device

1. Introduction

Discovery of ultrafast photo induced charge transfer at donor–acceptor (D/A) interface has brought a lot of interest in organic photovoltaic devices based on conjugated polymer and fullerene (C_{60}) [1–3]. The polymer-C_{60} bulk heterojunction concept is based on an active layer formed by bilayer deposition or a blend of electron donor polymer and acceptor C_{60} [4,5]. Upon absorption of photon; exciton dissociation occurs at the interface of donor and acceptor material. Ultrafast charge transfer of the electron from the conjugated polymer to the acceptor C_{60} leads to efficient charge separation. This charge transfer can only occur when the acceptor and donor are in close proximity typically less than 10 nm [6–8]. The close proximity of donor and acceptor can be achieved by using a blend of the two materials. The improvement of charge transport can be obtained by creating a concentration gradient of donor and acceptor within the active layer such that the donor rich phase is at anode and acceptor rich phase at the cathode [9].

It has been reported that V_{oc} and J_{sc} depend on inter-diffused active layer of the acceptor and donor. Variation of C_{60} and polymer layer thickness shows that within the examined thickness regime, the photocurrents in the inter-diffused devices increase with decreasing thickness as a result of improved charge transport out of the film [10]. Inter-diffused device has been fabricated by annealing at different temperature for different duration and effect of different heating temperature has been discussed [11,12]. Hence, it is very important to optimize the polymer/C_{60} layer thickness and annealing temperature and duration of annealing to get the optimum performance of D/A type of photovoltaic device.

Taguchi methodology is a very simple technique by which we can optimize device parameters within very less number of experiments [13–15]. This technique is based on "Orthogonal Array" experiments, which gives much reduced "variance" for the experiment with "optimum setting" of control parameter. A very useful statistical term "Signal to Noise ratios (*S*/*N*)", which is log function of desired output, serves to find out parameters which influences the most, to produce the desired parameters. The optimization involves determining the best control factor so that the output yields the targeted value. There are 3 types of signals-to-noise ratios (*S*/*N* ratio) for optimization: Smaller the Better, Larger the Better and Nominal the Best. Either of them

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Table 1
Orthogonal table according to Taguchi optimization with different combination of level of parameters used for device fabrication

Exp no.	C_{60} thickness (nm)	Thickness of P3OT (nm)	Annealing Temp. (°C)	Annealing time (min)	V_{oc} (V)	J_{sc} (mA/cm^2)	S/N ratio for V_{oc}	S/N ratio for J_{sc}
L1	110	45	50	5	0.30	0.6×10^{-4}	−10.45	−84.43
L2	110	100	120	15	0.34	1.04×10^{-4}	−9.37	−80
L3	110	135	180	30	0.25	0.25×10^{-4}	−12.04	−93.45
L4	145	45	120	30	0.40	1.2×10^{-5}	−7.95	−98.41
L5	145	100	180	5	0.29	0.4×10^{-5}	−10.75	−107.95
L6	145	135	50	15	0.25	0.5×10^{-5}	−12.04	−105.87
L7	220	45	180	15	0.39	1.0×10^{-5}	−8.17	−100
L8	220	100	50	30	0.29	1.6×10^{-5}	−10.75	−95.91
L9	220	135	120	5	0.23	0.52×10^{-5}	−12.76	−106.02

can be used for optimization depending upon the requirement of optimization.

1.1. S/N ratio for smaller the better (S–B)

This condition is used when we are interested in finding out the suitable parameters which could yield the desired lowest value of the targeted results from set of experiments giving range of results. The S/N ratio is calculated using the equation for "smaller the better".

$$S/N = -10\mathrm{Log}_{10}(1/n)\sum(y_i)^2. \quad (1)$$

Where y_i is the primary response and n is the number of repetitions of each experiment.

1.2. S/N ratio for larger the better (L–B)

This condition is used when from the set of experiments we desire to get information about those parameters which will give higher value of the targeted result. For example, if from a set of experiment the V_{oc} is in the range 0.1 V to 0.4 V and the desired result is higher than V_{oc} 0.4 V, then the S/N ratio is calculated using the equation for "larger the better"

$$S/N = -10\mathrm{Log}_{10}(1/n)\sum(1/y_i)^2. \quad (2)$$

In this paper we report our efforts to optimize different parameters of Poly (3-octylthiophene) (P3OT) and C_{60} heterojunction photovoltaic device with Taguchi optimization technique. Devices were fabricated with the optimized parameters and effects of different parameters were discussed.

2. Experimental

In this study regioregular Poly(3-octylthiophene) (Aldrich Ltd.), and C_{60} (Nanom Frontier carbon corporation) were used as purchased. Photovoltaic devices were fabricated with the structure ITO/C_{60}/P3OT/Au. Device parameters were selected according to the Taguchi optimization condition as given in Table 1. C_{60} films were thermally evaporated over ITO surface pre-cleaned with acetone and ethanol at better than 1×10^{-3} Torr pressure. P3OT layers were spin coated from 8.6 mg/ml chloroform solution by spin coating at 4000 rpm over the C_{60} layer. To complete the device structure Au contact (10–20 nm) over P3OT films were deposited by thermal evaporation at pressure better than 1×10^{-3} Torr. ITO and Au electrodes play the roles of electrons and holes collection in the device respectively as shown in Fig. 1 along with respective energy levels of the different layers. Fabricated C_{60}/P3OT bilayers were annealed in a furnace at different temperatures for different durations in argon atmosphere.

Thicknesses of the C_{60} and P3OT films were determined from optical density (OD) values which were calculated from transmission and reflection data measured with JASCO V-570 UV–VIS–NIR thin-film spectrometer system. The absorption coefficients used for calibrations are 14×10^4 cm^{-1} at 516 nm for P3OT and 6×10^4 cm^{-1} at 435 nm for C_{60} films. Absorption

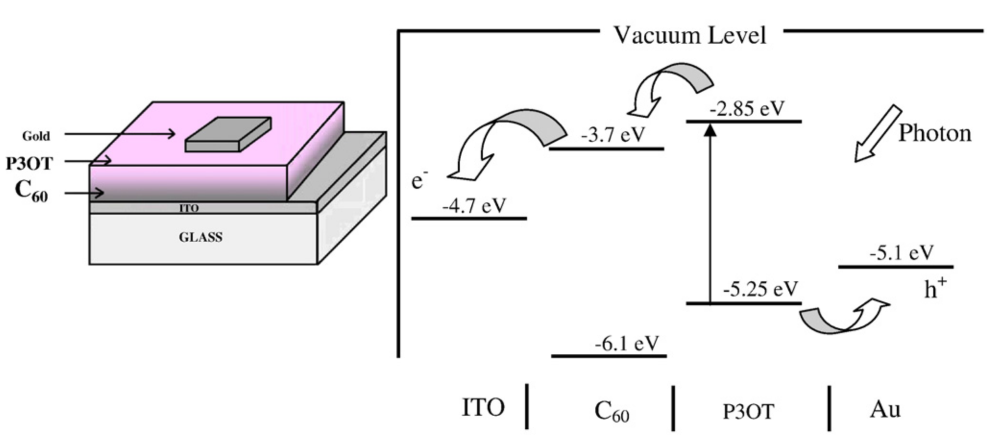

Fig. 1. Schematic diagram of fabricated devices with the structure ITO/C_{60}/P3OT/Au along with its respective energy levels.