International Journal of Advances in Engineering Research http://www.ijaer.com

(IJAER) 2014, Vol. No. 7, Issue No. III March **e-ISSN: 2231-5152, p-ISSN: 2454-1796**

INFLUENCE OF SOLVENT USED FOR SPIN COATING ON THE DEVICE PERFORMANCE OF SOLAR CELLS[1]

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ABSTRACT

One of the popular Solar cells, based on poly(3-hexylthiophene) (P3HT):TiO2 nanocomposite films are taken for this study. The influence of nanoparticle concentration, solvent used for spin coating, and the film morphology on the device properties was investigated. For low nanoparticle concentration (20–30%) the device performance was poor compared to pure P3HT, while for higher concentrations (50% and 60%) it shows a significant improvements. By changing the solvent (from chloroform to xylene) yields one to two orders of magnitude shows improvement in the nanocomposite photovoltaic cell efficiency. For optimal fabrication conditions, external quantum efficiency up to 15% and AM1 power conversion efficiency of 0.42% were obtained during the study.

The Organic/inorganic nanocomposites have several advantages over pure organic materials, such as high versatility since properties can be easily changed by varying composition and simplicity of achieving nanoscale sizes using self-assembly techniques, while the inherent advantages of organics technology, i.e., low cost production, low cost of the materials used, and possibility of fabrication of large area devices are preserved. Therefore, these materials are very promising for various devices such as light emitting diodes, photodiodes, photovoltaic cells, and gas sensors [1]. Applications of different organic–inorganic nanocomposites to organic solar cells [2–7] and organic light emitting diodes (OLEDs) [8,9] have been reported. Excellent performance of P3HT:CdSe nanocomposite solar cells with external quantum efficiency (EQE) over 54% and AM 1.5 power conversion efficiency of 1.7% was reported [6].

The External Quantum Efficiency upto 45% and power conversion efficiency of 0.49% was reported for PbS quantum dot sensitized organic solar cell with nanocrystalline TiO2 electrode. However, there are still many reports on composite devices with efficiency below 0.1% [2,5,7]. There have been several studies of the charge transport processes in organic–inorganic nanocomposites [10–13]. However, the reported results are contradictory. Both increase [13] and decrease [10] in mobility with increased nanoparticle concentration were reported.

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[1] How to cite the article:
Dileep P.; Influence of Solvent used for Spin Coating on the Device Performance of Solar Cells; *International Journal of Advances in Engineering Research*, June 2014, Vol 7, Issue 3, 54-60

The main reasons for this is, the differences in polymers and nanoparticles used, as well as differences in fabrication techniques, can account for observed differences in experimental results. The obtained results can deviate from theoretical predictions due to existence of phenomena such as local electrical field enhancement and different alignment of the chains affecting overall mobility due to high anisotropy of carrier mobility in conjugated polymers, which are not taken into account in commonly used transport models based on disordered hopping [10]. Furthermore, fabrication conditions, as well as type of nanoparticles and polymer, can significantly affect the film morphology and the device performance. While there have been studies investigating the influence of the film morphology in purely organic donor–acceptor blends on blend properties and organic optoelectronic device performance [14,15], systematic studies of the relationship between film morphology and its electrical and optical properties for organic–inorganic nanocomposites have been scarce [16].

In this work, we study the influence of different nanoparticle concentration and different solvent used on the performance of photovoltaic cells based on P3HT:TiO2 nanocomposites. The device structure was ITO/PEDOT:PSS (poly(ethylene dioxythiophene) blended with polystyrene sulfonic acid)/P3HT:TiO2/Al. ITO glass substrates with surface sheet resistance _10 X/_ were supplied by China Southern Glass Holding Co. Ltd., Shenzhen, China. PEDOT:PSS was obtained from Bayer AG, regioregular P3HT was purchased from Aldrich, and TiO2 nanoparticles with particle size 20–40 nm were purchased from Nanopowder Enterprises.

Thirty nanometer layer of PEDOT:PSS was then spincoated on ITO glass, followed by 24 h baking at 110 _C in a vacuum oven. After baking of PEDOT:PSS, _100 nm thick pure P3HT or P3HT:TiO2 films were spincoated.

The solutions for fabricating P3HT or P3HT:TiO2 films were prepared in a heated ultrasonic bath (at 50 _C) to increase solubility of P3HT. The films were baked in a vacuum oven for 24 h at 110 _C. The Al electrode was then evaporated in high vacuum. Pressure during evaporation was of the order 10_4 Pa. The current–voltage characteristics were measured using a Keithley 2400 sourcemeter. For white light efficiency measurements, Oriel 66002 xenon arc lamp with AM1 filter was used. The light intensity was 100 mW/cm2. For external quantum efficiency measurement, Oriel Cornerstone monochromator was used. Atomic force microscopy (AFM) measurements were performed using Digital Instruments Nanoscope III operating in tapping mode.

Figs. 1a and b show the current voltage characteristics and EQE for the composites with different P3HT:TiO2 ratios, respectively. The obtained AM1 power conversion efficiency was 0.06% for pure P3HT, 0.01% for 20% and 30% of TiO2, 0.08% for 40% of TiO2, 0.27% for 50% TiO2, 0.42% for 60% TiO2, and 0.07% for 70% TiO2. For low nanoparticle concentration, the cell performance is inferior to that of the pure P3HT, while for the TiO2 nanoparticle concentration of 50% and 60% considerable improvement in AM1 power conversion efficiency is obtained. For 70% TiO2 nanoparticle concentration, good quality uniform films could not be produced, so that the device performance worsens and the efficiency becomes comparable to that of pure P3HT. The low efficiency observed for nanoparticle concentration below 40% is possibly due to recombination of the separated charges. For TiO2:PPV poly (p-phenylene vinylene) composites with TiO2 concentration above 20 wt%, most excitons dissociated at the interface of the polymer and nanocrystals, but the charge collection efficiency was limited by recombination [11]. When the TiO2 concentration is low, isolated nanoparticles cause charge build up and prevent further charge transfer [18]. The electrons trapped at isolated nanoparticles or dead end conduction paths will eventually recombine with the holes in the polymer, lowering the efficiency of the device. With increased TiO2 concentration, electron transport through the nanocrystal network without recombination with the holes in the polymer becomes more likely. However, for very high nanoparticle concentration, the film quality deteriorates yielding inferior device performance. The best result was obtained for 60% TiO2, with open circuit voltage Voc ¼ 0:44 V, short circuit current density Isc ¼ 2:76 mA/ cm2, fill factor FF¼0.36, and efficiency g ¼ 0:42%. Fig. 2 shows I–V characteristics for P3HT:TiO2 cells with 60% nanoparticle concentration prepared from different solvents. The inset shows energy diagram of the device, with energy levels of PEDOT:PSS, P3HT, and TiO2 from [17–19]. It can be observed that the device performance is strongly dependent on the solvent used. The obtained AM1 power conversion efficiencies are 0.03% for chloroform, 0.09% for THF, 0.17% for chlorobenzene, and 0.42% for xylene. Open circuit voltage and fill factor show only weak dependence on the solvent used, while the short circuit current density was strongly affected by the solvent and it changed from 0.24 mA/cm2 for THF to 2.76 mA/cm2 for xylene. For 50% nanoparticle concentration, similar results were obtained, with g ¼ 0:002% for chloroform, 0.008% for THF, 0.13% for chlorobenzene, and 0.27% for xylene.

For pure P3HT films, however, no significant effect of solvent was observed and for all solvents used efficiency of 0.06–0.08% was obtained.

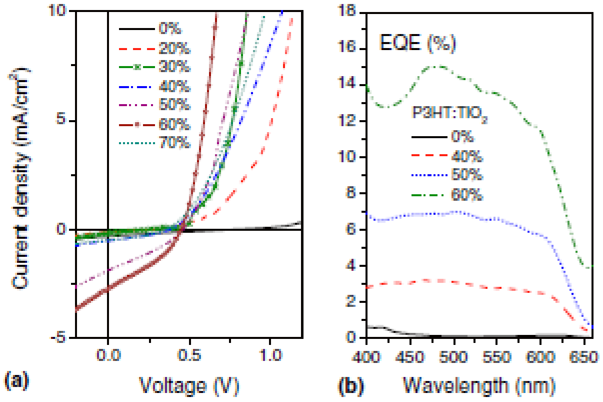

Fig. 1. (a) I–V characteristics for P3HT:TiO2 cells for different TiO2 concentration. Pure P3HT cell is also shown for comparison. (b) The comparison between external quantum efficiency (EQE) for nanocomposite and pure P3HT cells.

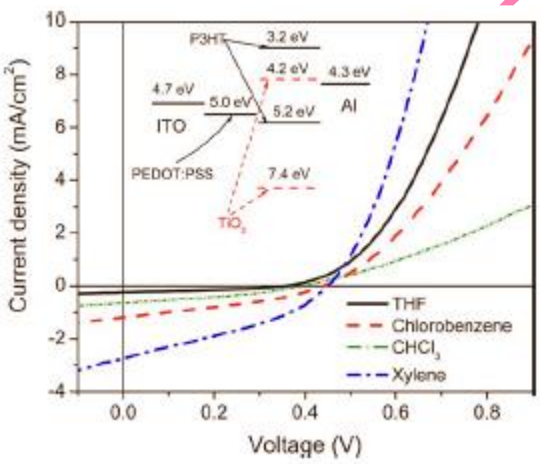

Fig. 2. I–V characteristics of P3HT:TiO2 cells with P3HT:TiO2 films spin-coated from different solvents. The inset shows the energy diagram of the devices.

In order to investigate the reasons for observed differences in the performance of the cells prepared from different solvents, we performed AFM (topography and phase contrast) measurements of the nanocomposite films. The obtained results for films with 60% TiO2 are shown in Fig. 3. The measurements were performed after baking the layers spin-coated on the top of baked PEDOT-PSS, i.e., same preparation conditions used for devices. The surface roughness is the lowest for chloroform (rms roughness of 22.9 nm) and the highest for xylene (rms roughness of 29.6 nm). However, more significant difference can be observed in phase contrast images. For the films prepared from xylene, the best mixing between TiO2 and P3HT is obtained, with large number of small domains yielding large interface and improved exciton dissociation. The obtained results are similar to those for poly(2-methoxy-5-(20-ethylhexyloxy)-1,4-phenylenevinylene) (MEH-PPV) and C60 composite films [15]. Liu et al. [15] explained the difference between the performance of the cells fabricated from xylene, dichlorobenzene, chlorobenzene, THF, and chloroform with preferential solvation of p-electron conjugated segments in aromatic solvents. However, while Liu et al. [15] obtained solvent dependent performance for pure MEH-PPV cells, our pure P3HT cells do not exhibit significant dependence on the solvent used for film fabrication, so that the explanation proposed by Liu et al. [15] is likely not applicable. However, it should be noted that the solvent evaporation rates influence the surface morphology of polymer films [20]. THF and chloroform have one order of magnitude higher vapor pressure compared to xylene [20], and hence evaporate significantly faster than xylene and chlorobenzene. In addition to solvent evaporation rate, the solvating power may significantly affect the morphology, since a good solvent could lead to a more extended polymer chain in solid state. Thus, a good solvent for P3HT with lower solvent evaporation rate may favor better mixing of the components resulting in improved exciton dissociation and short circuit current density.

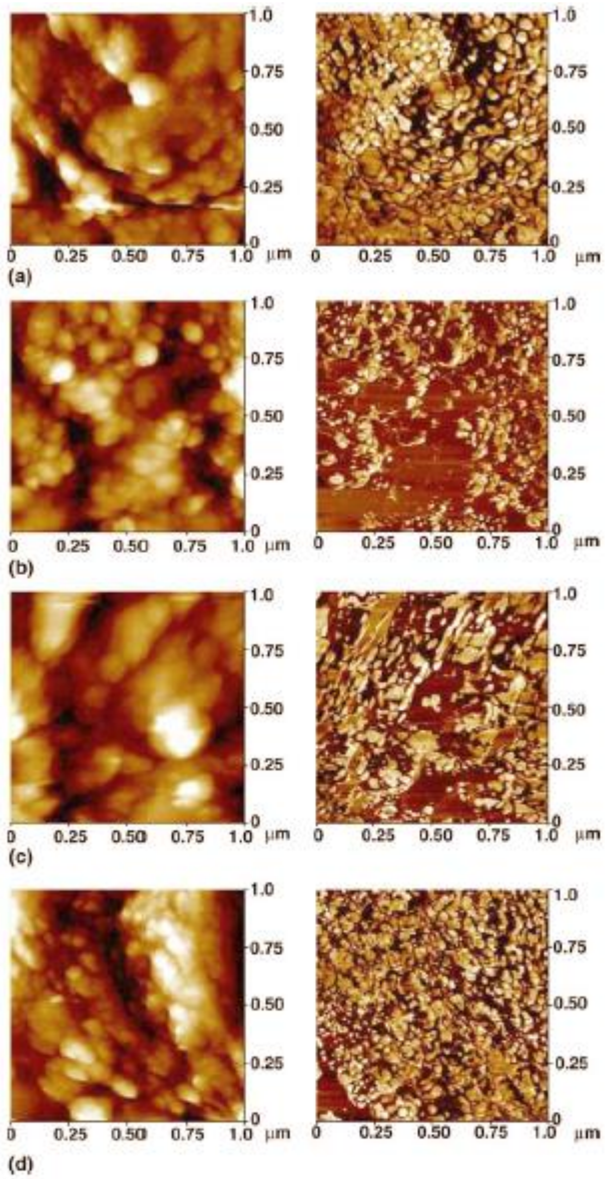

Fig. 3. AFM topography and phase contrast images of P3HT:TiO2 films spin-coated from different solvents: (a) chloroform, (b) THF, (c) chlorobenzene, (d) xylene.

To summarize, we have studied the performance of the P3HT:TiO2 nanocomposite solar cells as a function of TiO2 concentration and the solvent used for the film preparation. We found that the performance of cells with low (640%) and high (*P*70%) TiO2 concentration is comparable or worse than that of cells with pure P3HT, while for 50% and 60% TiO2 concentration significant improvements are obtained. We also found that solvents with lower vapor pressure such as xylene and chlorobenzene yield better mixing of TiO2 and P3HT and consequently better cell performance. The best performance was obtained for the cell with 60% TiO2 fabricated from xylene solution, with AM1 power con-version efficiency of 0.42%. The efficiency can be further improved by optimizing the film thickness, as well as encapsulation of the cells or measurements in inert atmosphere.

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