Nanoscale Charge Transport in P3HT:PCBM:Gold Nanoparticle Composite Materials for Polymer Solar Cell Application

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Introduction

In the past few years, conjugated polymer (CP) based photovoltaic devices have attracted a great deal of attention. In this work, we applied the various scanning probe techniques to characterize composite materials typically used to fabricate polymer solar cells: poly-3(hexylthiophene) (P3HT) and [6,6]-phenyl-C61-butyric acid methyl ester (PCBM) and P3HT/PCBM/Au nanoparticle samples (see Figure 1 for the chemical structures). The latter is studied due to the idea of using the gold nanoparticle surface plasmon to enhance the optical absorption of the composite films to increase the solar cell efficiency. Atomic force microscopy (AFM) is used to characterize the film morphology whereas conducting AFM is used to study the charge transport properties at the nanoscale (Figure 2). We found that annealing process lead to higher charge mobilities in all samples and higher solar cell efficiencies and there is a direct correlation between the nanoscale charge transport measurements and the device efficiencies.

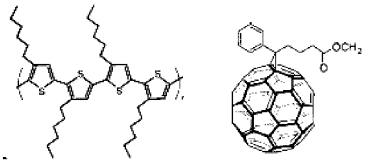

Figure 1. The chemical structures of materials used in this work.

Experimental

Sample preparation. All the films in this study were prepared using the same conditions as films used to fabricate the devices. Typically, powders of P3HT and PCBM were weighted and placed in a clean glass vial at the ratio of 1:0.8 by weight. Into this vial, chlorobenzene was added. A solution of gold nanoparticle capped alkyl thiol (5 nm in the diameter) at appropriate weight concentration was added into P3HT/PCBM solution to give 1:0.8:0.2 by weight of P3HT:PCBM:Au. Films prepared by spin coating these solutions onto pre-cleaned ITO-coated glass substrates.

Instrument. All AFM and C-AFM measurements were done in air under the ambient conditions and in the dark using the MultiMode (Veeco Inc.) with the controller IIIa.

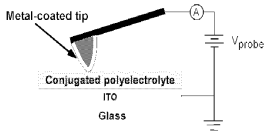

Figure 2. A schematic of C-AFM experimental setup for nanoscale charge transport measurements.

Results and discussion

Figure 3 shows the charge mobilities for as-cast and annealed P3HT, P3HT/PCBM, and P3HT/PCBM/Au films as measured by C-AFM using Pt probe. The current measured is contributed mainly by hole transport because the ITO and the Pt tip have high work functions of 4.7 eV and 5.6 eV, respectively. In all samples, the charge transport and mobility follow the space-charge current limited (SCCL) model ($J \sim V^2$) and the Poole-Frenkel law, respectively. Generally, annealing process helps to remove solvent residue, allows better polymer chain alignment and packing, and reduces the chain conformational distortion (twist, bend, etc.) therefore, annealing leads to higher charge mobility. Also, the addition of gold nanoparticles does not affect the hole mobility.

To correlate the nanoscale charge transport study to the bulk, solar cells were fabricated from P3HT/PCBM (labeled as control in Figure 2, bottom right) and P3HT/PCBM/Au (labeled as 5 nm particles). There is a direct correlation between the nanoscale charge mobility and the device efficiency: improving the charge mobility leads to devices with higher efficiencies. There is a direct correlation between the nanoscale charge mobility and the device efficiency: *improving the charge mobility leads to devices with higher efficiencies.*

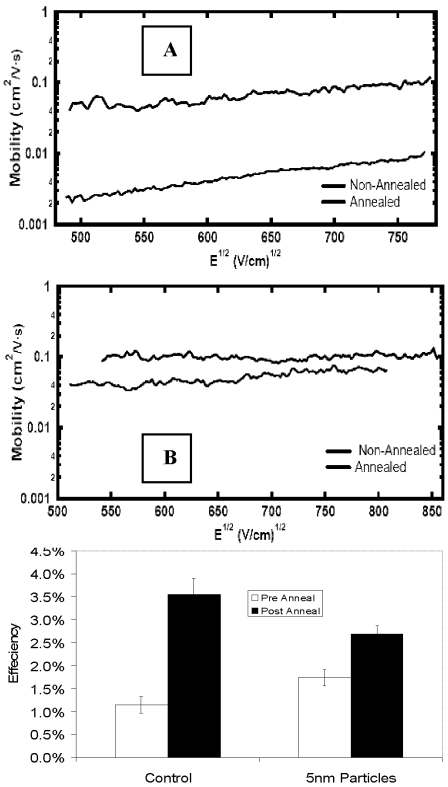

Figure 3. The charge mobilities for as-cast and annealed (A) P3HT/PCBM and (B) P3HT/PCBM/Au films; and the solar cell efficiencies (bottom) for as-cast and annealed P3HT/PCBM (control) and P3HT/PCBM/Au (5 nm particles).

For both sets of the devices, devices fabricated from annealed films have higher efficiencies than for devices fabricated from as-cast films. Comparing the as-cast devices, the P3HT/PCBM/Au device has higher charger mobility and efficiency than for the P3HT/PCBM device. For the annealed devices, although the charge mobility for the annealed P3HT/PCBM/Au is higher than for the annealed P3HT/PCBM film, the device efficiency is lower, 2.8% vs. 3.6%. The result is unexpected but the charge mobility measured here is for hole only whereas for real devices, both hole and electron mobilities are important in determining the device performance. We also measured the electron mobilities for all samples. For the P3HT/PCBM devices, the electron mobility for annealed device is higher than for unannealed one; however, the result is reversed for the P3HT/PCBM/Au devices. TEM images show that the gold nanoparticles aggregate to form large domains upon annealing. Possible reasons for the lower electron mobility are the trapping of electrons by gold nanoparticles [1,2] and/or the change in electron conduction path upon the gold nanoparticle aggregation.

Conclusions

In summary, the gold nanoparticles at low concentration and small size used in these studies increase the absorption of the composite films but do not improve the efficiency of the devices upon annealing due to the formation of large gold nanoparticle aggregations.

References

[1] Thomas, K. G.; Ipe, B. I.; Sudeep, P. K. *Pure Appl. Chem.* **2002**, *74*, 1731.

[2] Ipe, B. I.; Thomas, K. G.; Barazzouk, S., Hotchandani, S.; Kamat, P. V. *J. Phys. Chem.* **2002**, *106*, 18.