Applicability of Functionalized Pentacene in Photovoltaic Devices

D. Lehr, J.S. Brooks[1], J. Anthony[2]
Physics Dept. and NHMFL, Florida State University, Tallahassee FL 32310 US
Dept. of Chemistry, University of Kentucky, Lexington, KY 40506 US

Introduction

The conception of a cost effective way to produce clean energy to meet the demands of our high powered culture has become of ethical and economic importance to all sectors of society. The scientific community has especially been involved in searching for an alternative to conventional fossil fuel based energy and has largely looked to photovoltaics as the ideal choice. The high cost of producing Silicon or Gallium Arsenide based devices, however, reduces the affordability of energy from traditional solar cells. Because of this, a large interest has been formed around organic semiconducting materials due to their potentially low-cost production and versatility in device applications.

Of particular interest to this paper is the organic semiconducting crystal: Pentacene, which has been reported to have photo-excited conducting states[1]. The possible utilization of these states in photovoltaic devices is worth investigation.

It is thought that photo-excited states in functionalized Pentacene originate from the excitation of electrons in the Pentacene backbone that are subsequently trapped in the functional groups leaving behind depleted carriers which may be mobile. Hence, it seems sensible to use such a material as a p-type layer in a photovoltaic device.

Experiment

To be confident that the photo-effect reported in the single crystal by Brooks et al. is also present in a Pentacene thin film, the first part of this experiment was an investigation of thin film photo-excitation. A Pentacene film was grown by thermal evaporation to connect 4 separated terminals of ITO as shown in figure 1.

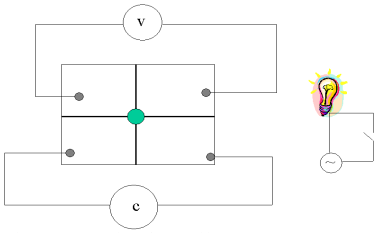

Figure1-setup for photo-effect measurement

A constant current of 1 nA was run across the sample while the potential difference was monitored. The sample was placed in a chamber isolated from outside light and the light inside was altered in a controlled manner.

After the photo-excited conducting states of Pentacene were observed in the thin film, 2 types of devices were fabricated to investigate the potential of the material for use in photovoltaics. The first device was made by growing a Pentacene film on top of ITO. The film was then doped in an iodine atmosphere for 18 hours. A TCNQ layer was then grown over top of a mask as the n-type layer. Aluminum was then deposited overtop of the same mask. Figure 2a shows the device layer by layer.

A second type of device was made in the same fashion, but before the Pentacene layer was grown, a PEDOT buffer layer was spin-coated onto the ITO. It has been shown that because of the potential energy barrier due to a difference in work function at an interface, a buffer layer can enhance device efficiency[2]. See figure 2c for a schematic of device type 2.

The completed devices were studied in low room light while a microscope light was turned on/off shining directly on the sample. The current was measured using an electrometer for a qualitative investigation of workability. IV characteristics were taken for devices of type 2.

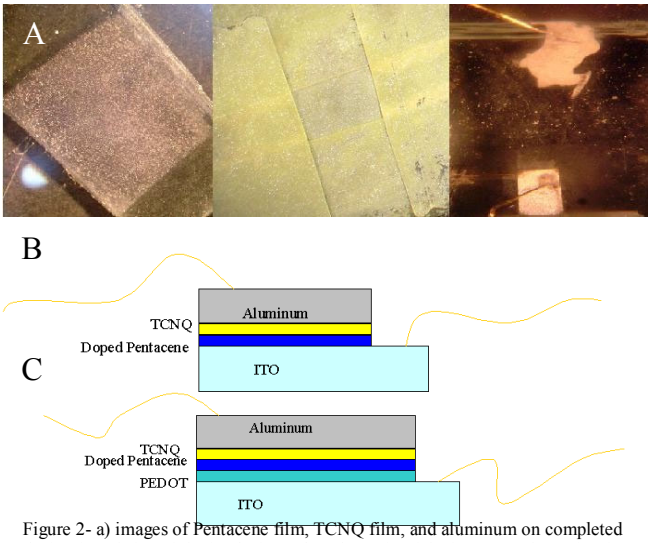

Figure 2- a) images of Pentacene film, TCNQ film, and aluminum on completed device from left to right for device 1. b) schematic of device 1. c) schematic of device 2.

Results and Discussion

In Figure 3 the effect of light on the conduction of a Pentacene thin film can be seen. The effect reported by Brooks[1] can be observed where light causes an immediate spike in conductance (probably due to the excitation of charge carriers) followed by a fast drop and subsequent exponential relaxation. Hence, it is feasible to generalize assumptions about the mechanisms of photo-excited states in single crystal Pentacene to thin films of TES-Pentacene.

Because it is believed that this change in conductance is a result of light exciting electrons into insulating channels, it was expected that Pentacene would make an ideal p-type material for photovoltaics. Further doping with iodine should also increase the number of charge carriers excited by photons in the material.

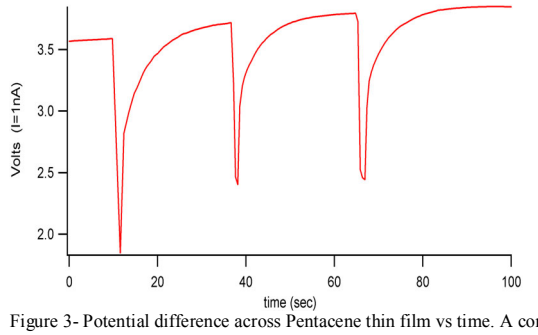

Figure 3- Potential difference across Pentacene thin film vs time. A constant current of 1 nA was maintained across the sample. Here the sample was placed in the dark. Every spike downward corresponds to light being turned on/off in less than a second.

A device of type 1 was fabricated and photo-induced current was measured across its two terminals for a qualitative investigation of workability. The device was approximately 6 mm^2 in area. When a bright light was shown on the sample, the current immediately jumped and quickly approached a steady value (see Figure 4). The peaks observed are correlated with how quickly the light is changed. (When light is increased or decreased slowly, a peak is not observed.) The current produced by the bright light was about 20 percent greater than the current produced by normal room light. The maximum steady current observed was only about .25 nA.

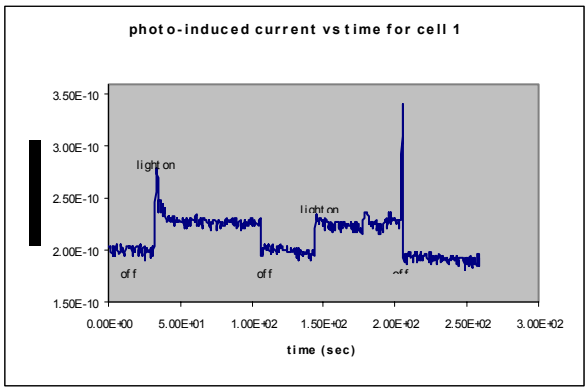

Figure 4- Current vs. Time for device 1. Bright light was turned on and off while the device was exposed to normal room light.

Better type 2 devices were made using a PEDOT buffer layer and a thinner TCNQ layer. These cells performed much better than type 1. The samples were examined in a similar manner to type 1 samples for a qualitative comparison. As can be seen in figure 5a, much higher currents were produced by type 2 devices.

When the IV characteristics of the devices were investigated, open circuit voltages as high as 432 mV and short circuit currents of 95.7 nA. were observed from a device measuring approximately 15 mm^2 in area. These devices were very temperature dependent as can be seen in the contrast between figures 5b and 5c. When the sample was subjected to high light levels at room temperature (see figure 5b), the IV characteristics were much less desirable then when the sample was subjected only to room light at approximately 100 ^{o}C (see figure 5c).

It has been understood that charge carriers in organic materials can experience states of thermally activated mobility[3]. This is most likely the origin of the temperature dependent IV characteristics of these devices; however because of the possibilities associated with a device that can produce thermally triggered excitons, a non transparent device was made to test the possibility of the phonon taking the place of the photon in these cells. Unfortunately, no EMF was detected and it was concluded that for this configuration, a thermally induced internal electric field cannot be produced. Figure 6 is a schematic of the device that was tested.

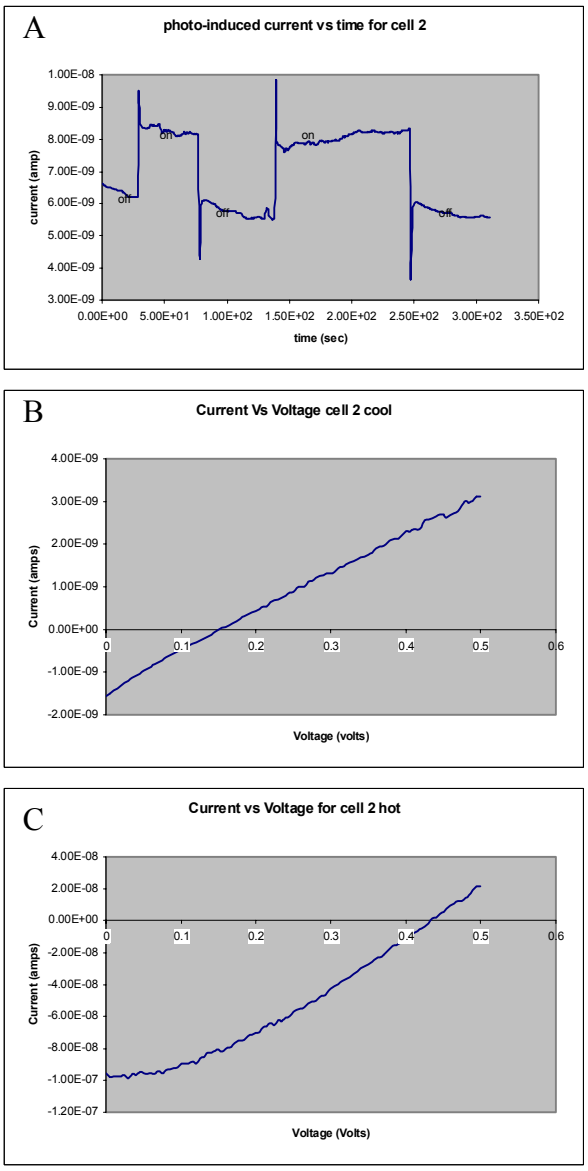

Figure 5- a) Light on/off experiment done for comparison with figure 4 b) typical room temperature IV curve for sample of type 2 . c) Typical IV curve for type 2 at 100 C.

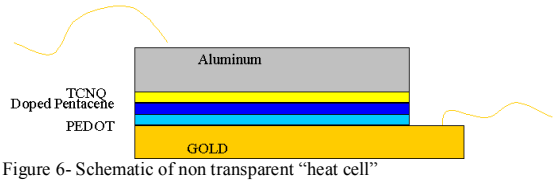

Figure 6- Schematic of non transparent "heat cell"

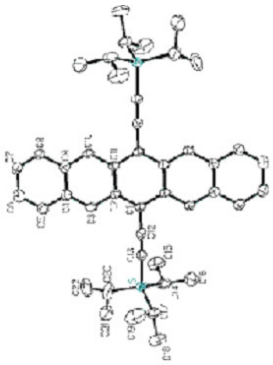
Figure 7- an example of functionalized pentacene

Conclusions

It appears that iodine-doped Pentacene is not such an ideal material for use in photovoltaics. This may be because of misinterpretation of the photo-effect observed in Pentacene. If the charge carriers produced in Pentacene by light are in fact electrons instead of holes, then the iodine doping done in this experiment may have been partly canceled by the photo-effect instead of being added to. Better quality films may also prove to yield more efficient devices. Also, while heating seems to be nothing more than a way to increase mobility in the devices discussed here, the advantages of a mechanism that would be able to convert thermal energy to electricity make further investigation into this possibility nearly essential. If such a phenomenon were realized, many active layers could be stacked in a series without regard to transparency. Solar heating could then be used to activate the device.

Acknowledgements

This research was supported by the National Science Foundation through the REU Program. Many of the supplies were provided by the Brooks Condensed Matter Research group at the National High Magnetic Field Laboratory (supported by NSF-DMR and DARPA-DSO). This research was also made possible by the Center for Integrating Research and Learning at the National High Magnetic Field Laboratory.

References

[1] J.S. Brooks, T. Tokumoto, E-S Choi, D. Graf, N.Biskup, D.L. Eaton. Persistent photo-excited conducting states in functionalized Pentacene. J. Appl. Phys. In press.
[2] I. Yoo, M. Lee, C. Lee, D-W. Kim, I.S. Moon, D-H. Hwang. The effect of a buffer layer on the photovoltaic properties of solar cells with P3OT: Fullerene Composites. ICSM 2004 Wollongong Aust. To be published.
[3] V. Dyakonov, J. Parisi, D. Chirvase, I. Riedel. Realisation of polymer-fullerene solar cells with low recombination losses. ICSM 2004 Wollongong Aust. To be published.