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# Performance Characteristics of Organic Photovoltaic Cells with Pentacene as a Hole Transport Layer

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*We have investigated the dependency of power conversion efficiency on deposition rate, substrate temperature, and post annealing during fabricating pentacene-based PIN photovoltaic cells with a structure of ITO/poly (3,4-ethylenedioxythiophene)-poly (styrene sulfonate)(PEDOT: PSS)/pentacene/pentacene: C<sub>60</sub>/C<sub>60</sub>/2,9-dimethyl-4,7-diphenyl-1,10-phenanthroline (BCP)/Al. The maximum power conversion efficiency of pentacene-based photovoltaic cells has been achieved to be 2.25% by adjusting process parameters such as deposition rate (0.2 Å/s), substrate temperature (60°C), and post annealing (200°C). The effects of these parameters are elucidated from the device performance characteristics such as open-circuit-voltage ( $V_{oc}$ ), short-circuit-current ( $J_{sc}$ ), and fill factor ( $FF$ ).*

**Keywords** Deposition rate; organic photovoltaic cell; pentacene; PIN; post annealing; substrate temperature

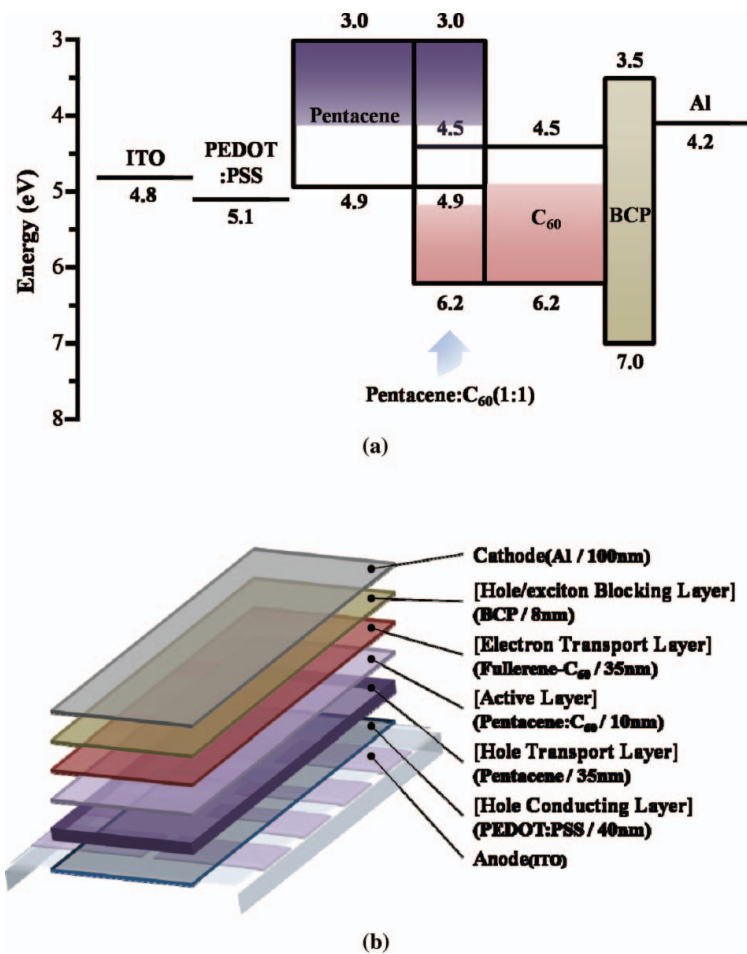
## Introduction

Pentacene thin film has been extensively studied as a hole transport layer in organic photovoltaic cells [1–14] because the advantages offered by pentacene are attributed to good semiconducting behavior such as high mobility ( $\sim 1.5 \text{ cm}^2/\text{Vs}$ ) [15–20], long exciton diffusion length ( $65 \pm 16 \text{ nm}$ ) and well suited absorption spectrum in the solar spectrum [1,21–23]. However, pentacene-based photovoltaic cells have been reported with relatively minor photovoltaic response.

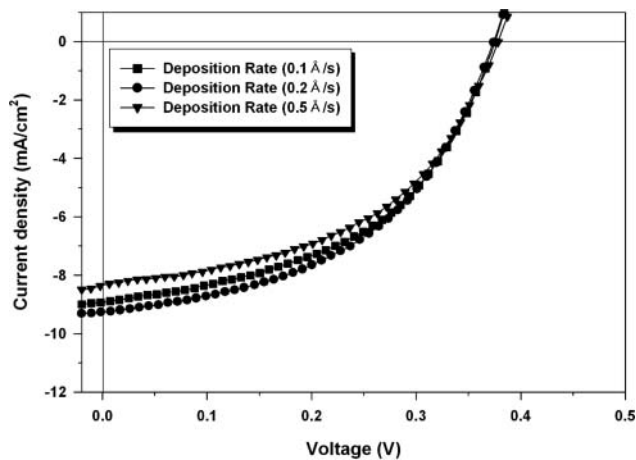
In this study, we have investigated the effects of various deposition conditions which are contributed to the properties of pentacene thin film such as deposition rate [24], substrate temperature [25], and post annealing [26,27] on the power conversion efficiency of pentacene-based PIN photovoltaic cells with a structure of ITO/poly (3,4-ethylenedioxythiophene)-poly (styrene sulfonate)(PEDOT: PSS, 40 nm)/pentacene (35 nm)/pentacene: C<sub>60</sub> (10 nm)/C<sub>60</sub> (35 nm)/2,9-dimethyl-4,7-diphenyl-1,10-phenanthroline (BCP, 8 nm)/Al (100 nm).

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**Figure 1.** Pentacene-based photovoltaic cells with PIN structure: (a) energy level diagram and (b) schematic device structure.



**Figure 2.** J-V characteristics of pentacene-based photovoltaic cells fabricated at various deposition rates.

## Experimental

### Materials

PEDOT:PSS was purchased from (Baytron P from H. C. Starck GmbH) and was used as a hole conducting layer material. Pentacene (formula:  $C_{22}H_{14}$ , molecular weight: 278.35 g/mol, melting point: 372–374°C) and  $C_{60}$  (formula:  $C_{60}$ , molecular weight: 720.64 g, melting point: >280°C, Tg: 174°C) were used as a donor and an acceptor,

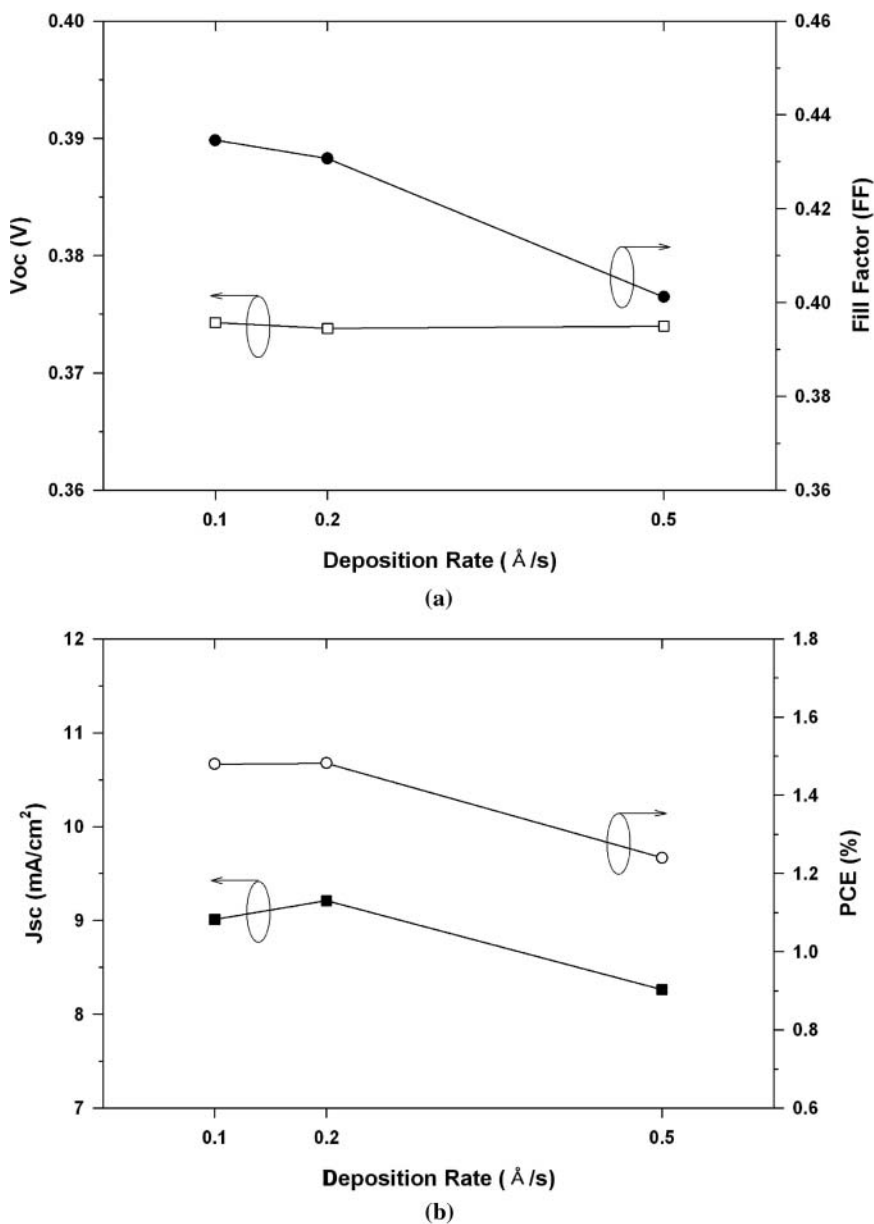


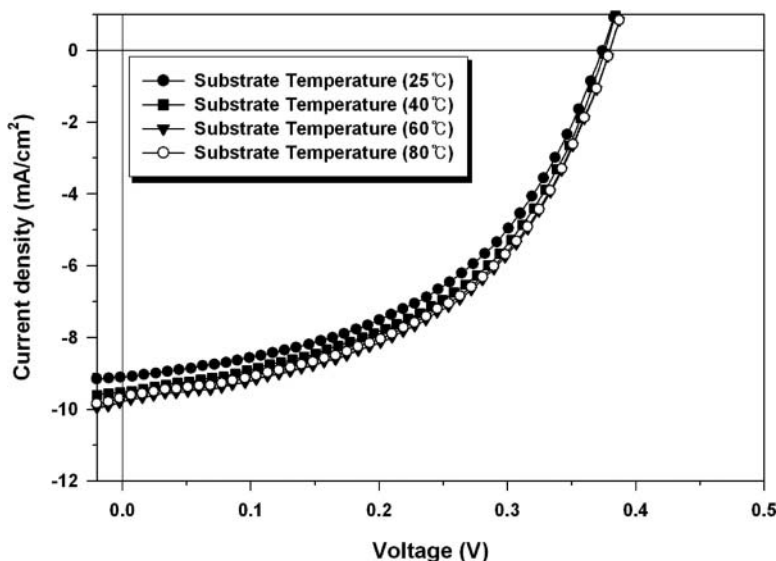
Figure 3. Photovoltaic response of the devices fabricated at various deposition rates.

respectively. Twice sublimed pentacene (99.99%) and C<sub>60</sub> (99.5%) were purchased from Sigma-Aldrich. As hole/exciton blocking layer material, bathocuproine (BCP, formula: C<sub>26</sub>H<sub>20</sub>N<sub>2</sub>, molecular weight: 360.46 g/mol, melting point: 277–285°C, Acros Organics) was used. Aluminum (formula: Al, molecular weight: 26.98 g/mol, melting point: 660.30°C, boiling point: 2467.00°C) as a cathode was purchased from CERAC, Inc.

### *Fabrication of Pentacene-Based Photovoltaic Cells*

The patterned ITO glass substrates were cleaned with acetone, ethanol and isopropyl alcohol for 30 min by sonication, and then the samples were rinsed by ethanol. Pre-cleaned ITO surface was spin-coated with PEDOT: PSS solution. Before spin coating, PEDOT: PSS solution was filtered using a 0.45 μm Millipore polytetrafluoroethylene (PTFE) syringe filter. Spin-coated thin film was dried on the hot plate at 120°C for 10 min in air. The thickness of PEDOT: PSS film was controlled to be 40 nm.

Photovoltaic cells based on PIN heterojunctions have been fabricated via thermal evaporation in a high vacuum chamber with a base pressure of  $\sim 2 \times 10^{-7}$  torr for a structure of ITO/PEDOT: PSS/pentacene/pentacene: C<sub>60</sub>/C<sub>60</sub>/BCP/Al. By thermal evaporation, a homogeneous layer with well-controlled thickness and deposition rate were obtained. Pentacene thin film (35 nm), pentacene: C<sub>60</sub> thin film (10 nm), C<sub>60</sub> thin film (35 nm), and BCP thin film (8 nm) were sequentially deposited onto the PEDOT: PSS thin film, followed by a 100 nm thick Al cathode, which was evaporated through a shadow mask. For pentacene layer, we optimized deposition conditions such as deposition rate and substrate temperature. Post annealing was performed at various temperatures for 1 min in vacuum. The energy level diagram and the device structure of pentacene-based photovoltaic cells are shown in Fig. 1.



**Figure 4.** J-V characteristics of pentacene-based photovoltaic cells fabricated at various substrate temperatures.

## Measurements

The thicknesses of PEDOT:PSS thin film were controlled by the digitalized rpm system in spin coater (MS-A100, Mikasa Co. Ltd) and were measured using a scanning electron microscope (SEM)(HITACHIS-4200). These of deposited organic and cathode materials were measured using a well calibrated quartz crystal thickness monitor (CRTM-600, ULVAC kiko Co. Ltd.) with thermal evaporator (VPC-260, ULVAC kiko Co. Ltd). The J-V characteristics and power conversion efficiencies were measured using a multi-source

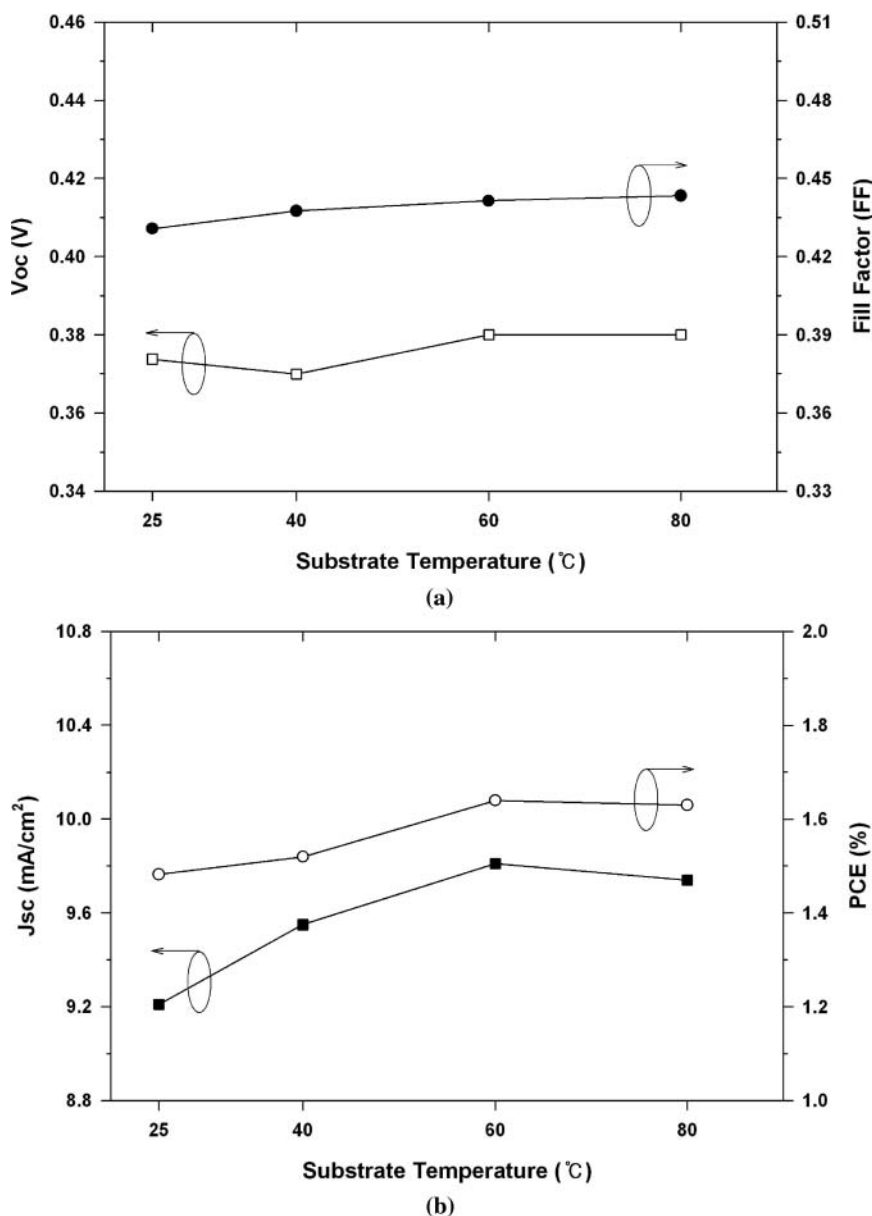


Figure 5. Photovoltaic response of the devices fabricated at various substrate temperatures.

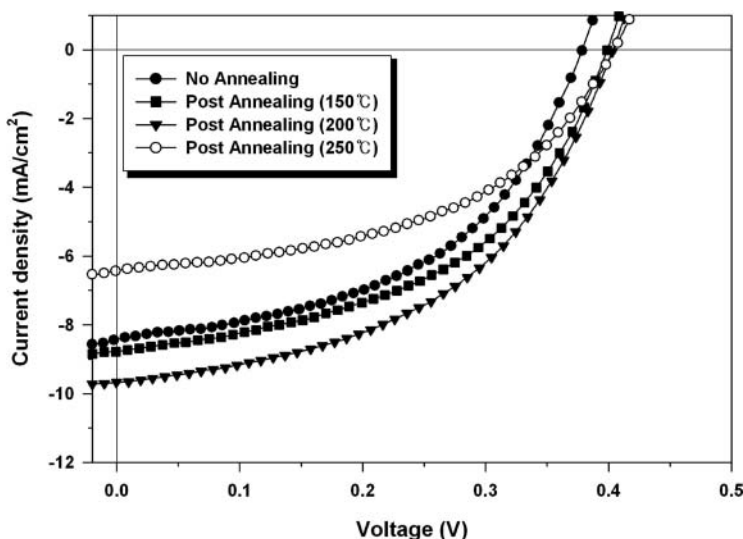
meter (KEITHLEY 2400) and a solar simulator (XES 301S, SAN-EL Electronics). The Xenon lamp ( $100 \text{ mW/cm}^2$ ) was used as a light source. The illumination intensity has been measured by a silicon photo-diode calibrated for an AM1.5 spectrum.

## Results and Discussion

The J-V characteristics and photovoltaic responses of pentacene-based photovoltaic cells with various deposition rates are shown in Figs. 2 and 3. As the deposition rate of pentacene increased, a fill factor (FF) value decreased. A higher value of short-circuit current density ( $J_{sc}$ ) of the devices was obtained at the deposition rate of  $0.2 \text{ Å/s}$ . When pentacene thin film was deposited at  $0.2 \text{ Å/s}$ , the power conversion efficiency of 1.48% was achieved. In general, the grain size is strongly dependent on deposition rate: the faster the deposition rate, the smaller the grain size and the higher the number of grain boundaries [28]. Additionally, the degree of disorder and defects in the thin film increases with faster rates. Therefore, the poor morphologies by faster rates cause decreased FF values. However, it is supposed that a suitable deposition rate for pentacene thin film contributes to the growth of pentacene/ $C_{60}$  interface and leads to the enhancement of the power conversion efficiency on the photovoltaic cells.

Figures 4 and 5 show the J-V characteristics and photovoltaic responses of pentacene-based photovoltaic cells with various substrate temperatures, respectively. We demonstrated power conversion efficiency of 1.63% from the device with a pentacene thin film in which substrate temperature was adjusted to  $60^\circ\text{C}$  and deposition rate to  $0.2 \text{ Å/s}$ . An open-circuit voltage ( $V_{oc}$ ) and FF values of pentacene-based devices have no dependency on the substrate temperature. It was reported that substrate temperature for pentacene thin films has influenced on hole mobility by improved grain size [25]. A proper substrate temperature for pentacene thin films leads to the enhancement of  $J_{sc}$  values because of high hole mobility with large grain size. It is known that pentacene possesses crystalline nature.

Performance characteristics of pentacene-based photovoltaic cells after post annealing treatment, are presented in Figs 6 and 7. The power conversion efficiency of 2.25% has



**Figure 6.** J-V characteristics of pentacene-based photovoltaic cells treated by post annealing.

been achieved from the device in which deposition conditions were optimized as described above and thermal annealing was performed at 200°C for 1 min in vacuum. Typically, the devices after post annealing treatment have enhanced performance characteristics because of increase in the charge carrier mobility as a result of enhanced crystallization [26,27]. After post thermal annealing, increased values of  $V_{oc}$ , FF and  $J_{sc}$  significantly affect on improving power conversion efficiency in this study.

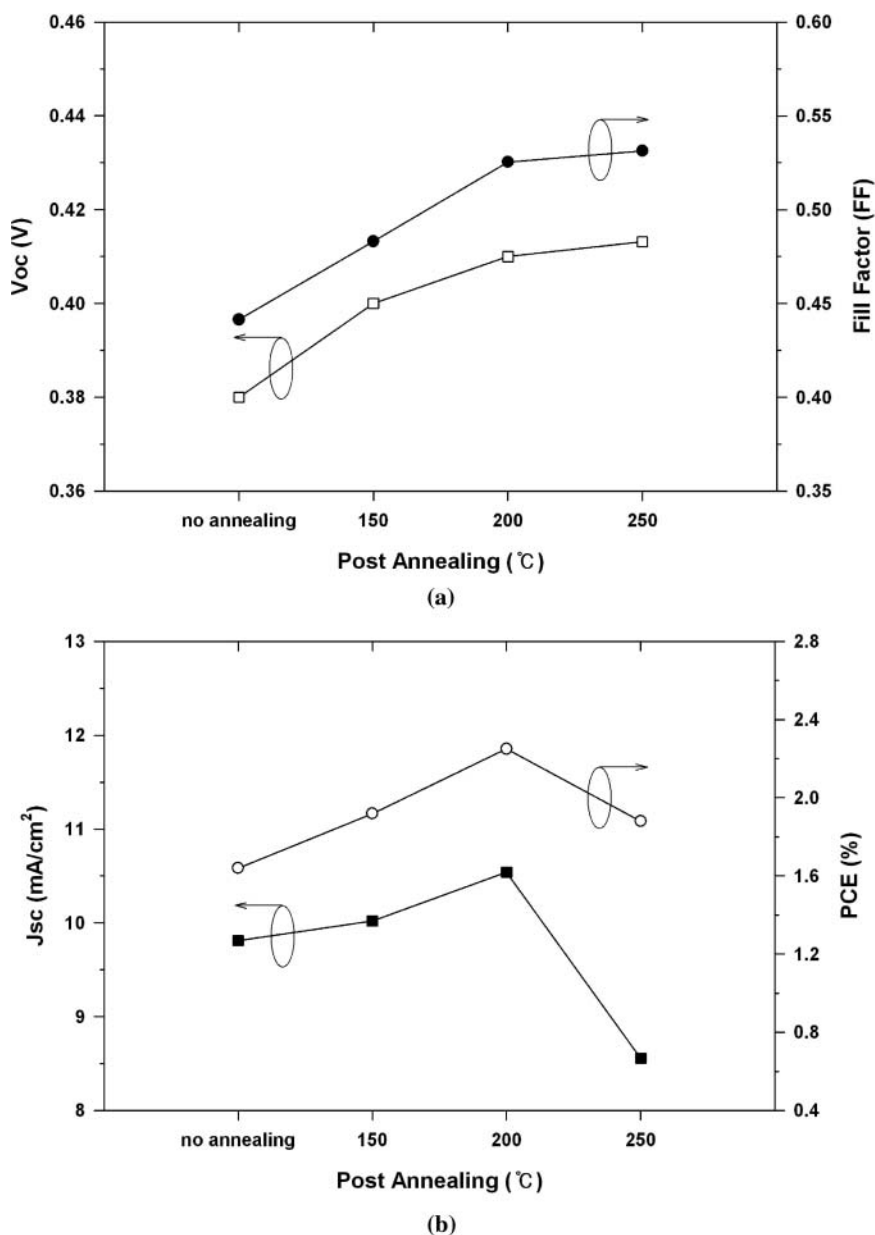


Figure 7. Photovoltaic response of the devices treated by post annealing.



## Conclusions

We have fabricated pentacene-based photovoltaic cells based on PIN heterojunctions to demonstrate the dependency of power conversion efficiency on deposition rate, substrate temperature, and post annealing.  $V_{oc}$  values of pentacene-based devices have no dependency on the deposition rate and the substrate temperature and increase with thermal annealing. These performance characteristics were determined by  $J_{sc}$  rather than  $V_{oc}$ . As these parameters lead to enhancement of  $J_{sc}$ , the power conversion efficiency of the devices increased. Because of the crystalline nature of pentacene, the current photovoltaic cells are strongly influenced by post annealing treatment after device fabrication in vacuum.

## Acknowledgment

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