Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Electronic Supplementary Information (ESI)

Vertical Phase Separation of Conjugated Polymer and Fullerene Bulk Heterojunction Film Induced by High Pressure Carbon Dioxide Treatment at Ambient Temperature

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This file includes:

1. A comparison of each element's SIMS profile

To ensure that SIMS sulfur profiles represent P3HT concentrations and the rest of the blend can be considered to be PCBM, each element's profile of a 96 hour treated film is compared in Figure S1. While sulfur was used to tag P3HT, oxygen could be used to tag PCBM as well. The trend of the sulfur profile shows the opposite trend of the oxygen profile. Therefore, the PCBM concentration can be estimated by P3HT concentration indicated by the sulfur SIMS profile.

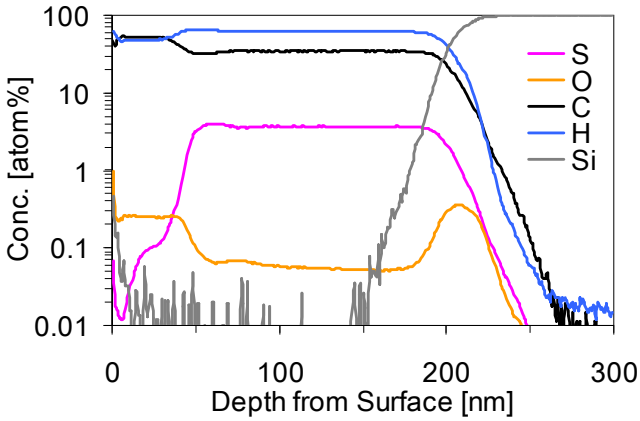

Figure S1 Each element's SIMS profile in 96 hour treated film.

2. XPS measurement

To estimate P3HT occupancy, the C/S atomic ratios ($r_{C/S}$) were evaluated using the following equation:

$$r_{C/S} = \frac{I_C / S_C}{I_S / S_S} \quad (1)$$

where I is the peak area and S is the atomic sensitivity factor, and each suffix corresponds to each element respectively. The integrated areas of the XPS peaks were calculated using XPSPEAK41 software and the Shirley method was used to subtract the background. The atomic sensitivity factors were extracted from the empirical values reported by Wagner et al..[1] Assuming that $r_{C/S}$ = 10 in pristine P3HT film, the surface occupancies of P3HT on each P3HT:PCBM blend film were estimated.

The calculated surface occupancies of P3HT on the surface of the P3HT:PCBM films are approximately 63% in the as cast film, 25% in the 48 hour treated film, and 1% in the 96 hour treated film. Although the calculated numbers contain some errors due to contamination of CO_2 to which the sample was exposed during treatment and an instrumental difference of sensitivity factors, the revealed trend is obvious enough so that those errors does not affect to the conclusion.

3. Original SEM images

Figure S2a and S2b are original cross sectional images of Figure 2a and 2b respectively. These have been trimmed and rotated. Scale bars have been inserted according to originally displayed ones. The texture seen on the fractured surface of silicon substrate is sputtered gold.

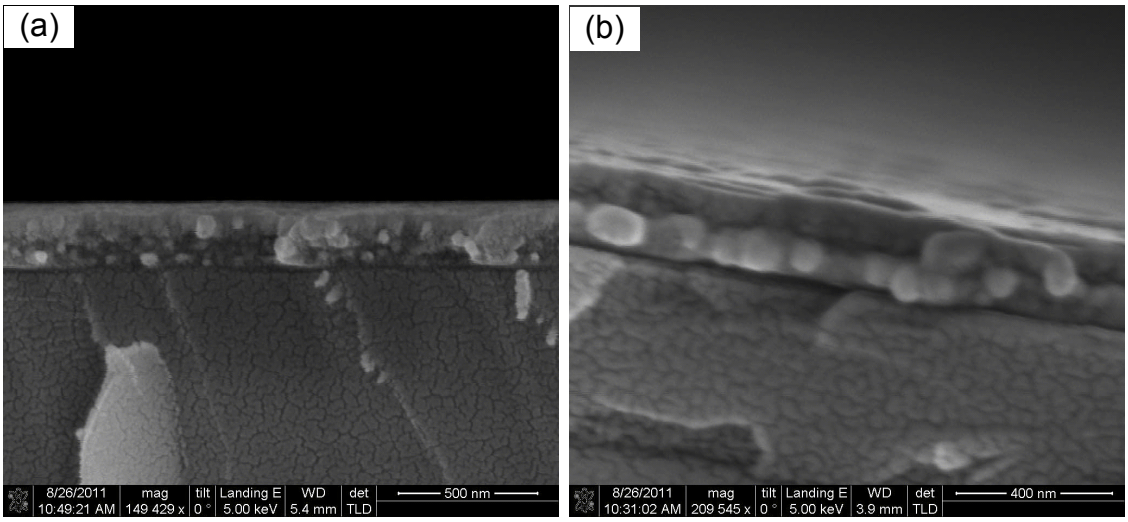

Figure S2 The original images of cross sectional SEM shown as Figure 2a and 2b in the body. (a) As cast. (b) After 96 hour CO_2 treatment.

4. Peak positions of emission spectra

Peak positions of emission spectra shown in Figure 3 have been extracted in Figure S3. Results of 2 hour and 72 hour treated film have been added. Emission spectra can indicate solar cell performance.

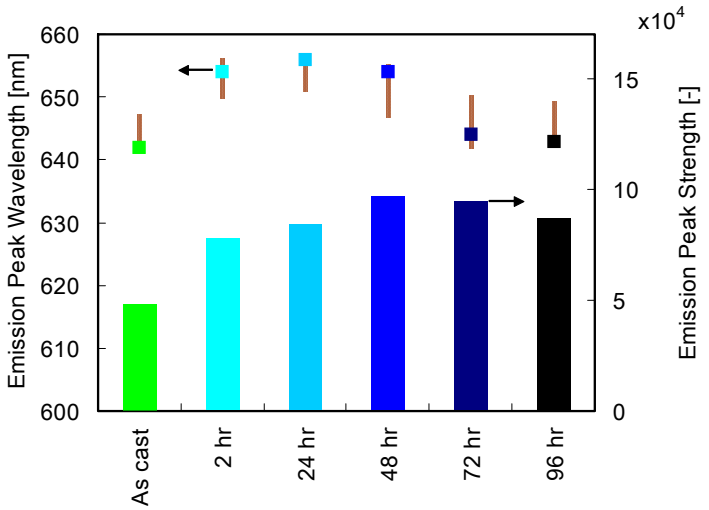

Figure S3 The peak positions of emission spectra shown in Figure 3. The peak wavelengths have been shown with the range that the strength difference from the peak is less than 1 %.

Reference

[1] C. D. Wagner, L. E. Davis, M. V. Zeller, J. A. Taylor, R. H. Raymond, L. H. Gale, *Surf. Interface Anal.*, 1981, **3**, 211.