Molecular structure analysis in solution-processed pentacene films by photoconversion reactions

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Pentacene (PEN; Figure 1a) is a semiconductor material used as an active layer for organic field-effect transistors (OFETs) [1]. To develop solution-processed OFETs, Yamada and co-workers developed 6,13-dihydro-6,13-ethanopentacene-15,16-dione (PDK; Figure 1b), which is a solvent-soluble precursor compound of PEN. This compound can be photochemically converted to the target material in thin films [2], and the photoconversion reaction can be accelerated by adding 1,2,4-trichlorobenzene (TCB) to the precursor film [3]. Nevertheless, the presence of residual TCB in the precursor film has not been confirmed so far, suggesting that a more detailed analysis of the precursor method is needed. In this study, infrared p-polarized multiple-angle incidence resolution spectrometry (pMAIRS) [4] is employed to analyze the effect of additives on the conversion ratio of PDK to PEN. In addition, the molecular aggregation structure in the photoconverted pentacene films is analyzed by using the two-dimensional grazing incidence X-ray diffraction and atomic force microscopy techniques.

(a) (b)

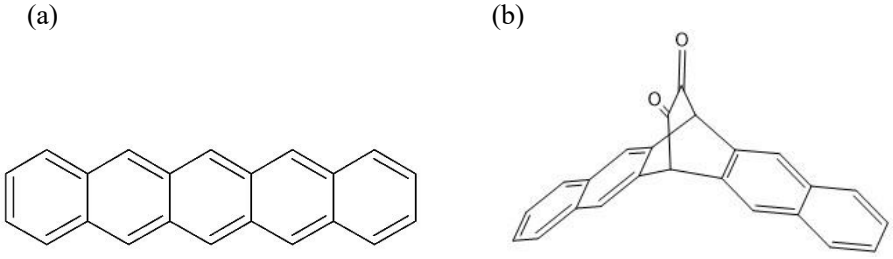

Figure 1 Chemical structures of pentacene (a) and 6,13-dihydro-6,13-ethanopentacene-15,16-dione (b).

[1] Lin, Y. Y. et al. *IEEE Electron Device Lett*. **1997**, *18*, 606. [2] Yamada, H. et al. *Chem. Eur. J.* **2005**, *11*, 6212. [3] Nakayama, K. et al. *J. Mater. Chem. C* **2013**, *39*, 6244. [4] Hasegawa, T. et al. *Bull. Chem. Soc. Jpn.* **2020**, *93*, 1127.