## Analysis of Photoconversion Reaction in a Pentacene Precursor Film Kyoto Univ.<sup>1</sup>, NAIST<sup>2</sup> °Tao Fang<sup>1</sup>, Nobutaka Shioya<sup>1</sup>, Kazutaka Tomita<sup>1</sup>, Mariko Yoshida<sup>1</sup>, Takafumi Shimoaka<sup>1</sup>, Hironobu Hayashi<sup>2</sup>, Hiroko Yamada<sup>2</sup>, Takeshi Hasegawa<sup>1</sup> E-mail: fang.tao.58x@st.kyoto-u.ac.jp

Pentacene (PEN, Figure 1(a)) is used as an active layer for organic field-effect transistors (OFETs) [1]. Since this compound is essentially insoluble in most solvents, thin films are generally prepared by vacuum deposition [2]. To develop solution-processed OFETs, Yamada and co-workers synthesized 6,13-dihydro-6,13-ethanopentacene-15,16-dione (PDK, Figure 1(b)) [3], which is a soluble precursor compound of PEN. This compound can be photochemically converted to PEN in thin films, which exhibit a field-effect mobility comparable to that of vapor-deposited films [4]. Nevertheless, the film quality in terms of crystallinity and grain size is significantly low, which requires a more detailed analysis of the molecular aggregation structure. In this study, infrared p-polarized multiple-angle incidence resolution spectrometry (pMAIRS) [5] and two-

dimensional grazing incidence X-ray diffraction (2D-GIXD) are employed to analyze the molecular aggregation structure in the photoconverted PEN film. The combination of 2D-GIXD and pMAIRS has readily revealed that the photoconversion product (PEN) exhibits crystalline polymorphism in the films, in which the so-called bulk phase is the major component.



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] Someya, T. et al. *Proc. Natl. Acad. Sci.*2005, *102*, 12321. [3] Yamada, H. et al. *Chem. Eur. J.* 2005, *11*, 6212. [4] Nakayama, K. et al. *J. Mater. Chem.*C 2013, *39*, 6244. [5] Hasegawa, T. et al. *Bull. Chem. Soc. Jpn.* 2020, *93*, 1127.