NEXAFS-Study on Thermal Degradation of PM6:Y6 Organic Solar Cell Active Layers

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In recent years, environmental and energy issues such as global warming and the depletion of fossil fuel resources have become increasingly serious, leading to growing worldwide interest in renewable energy, including solar power generation. Among various photovoltaic technologies, organic solar cells (OSCs) have attracted considerable attention as next-generation solar cells because of their advantages, such as low cost, light weight, and mechanical flexibility. Currently, the power conversion efficiency of OSCs has improved to around 20%, which is comparable to that of conventional silicon-based inorganic solar cells[1]. However, their long-term stability remains a significant challenge.

Due to the intrinsic properties of organic materials, OSCs are susceptible to degradation caused by various external environmental factors, such as light, heat, oxygen, and moisture, resulting in performance deterioration. In particular, under actual operating conditions, solar cells are exposed to high temperatures due to continuous solar irradiation, making thermal degradation unavoidable. Nevertheless, the effects of thermal stress on the active layer structure and the donor/acceptor interface[2], as well as the underlying degradation mechanisms, have not yet been fully clarified. Therefore, a detailed understanding of the thermal degradation process in OSCs is essential for their practical application.

Previous studies have suggested that thermal degradation mainly originates from changes in the phase-separated structure and crystallinity of the active layer. However, under high-temperature conditions, possible changes in the molecular backbone and functional groups cannot be ruled out. In this study, to clarify the origin of thermal degradation in the widely used PM6:Y6 system, near-edge X-ray absorption fine structure (NEXAFS) measurements were carried out at BL-13 of HiSOR.

In the experiments, solutions of PM6, Y6, and a PM6:Y6 blend were spin-coated onto Au substrates to prepare thin-film samples, and their NEXAFS spectra were measured. The samples were then thermally aged by heating them on a hot plate at 150 ° C for 24 hours. After thermal treatment, NEXAFS spectra were measured again and compared with those obtained before heating to investigate thermally induced degradation. As an example, the C 1s NEXAFS spectra of pristine Y6 and thermally aged Y6 are shown in Figure 1. The spectra reveal differences in polarization dependence before and after thermal treatment, indicating that a change in molecular orientation occurred in Y6.

The results of this study demonstrate that the degree of thermal degradation differs between PM6 and Y6. While PM6 shows no significant change, Y6 exhibits a pronounced change in molecular orientation. This difference is considered to originate from the disparity in glass transition temperatures between PM6 and Y6[3]. Furthermore, in the PM6:Y6 blend film, the possibility of intramolecular twisting in Y6 molecules was suggested[4].

These findings indicate that thermal degradation involves both orientation changes associated with the glass transition temperature and structural changes in the molecular backbone, such as intramolecular twisting. This provides a new perspective on thermal degradation mechanisms, extending beyond the conventional understanding that thermal degradation is primarily governed by physical changes.

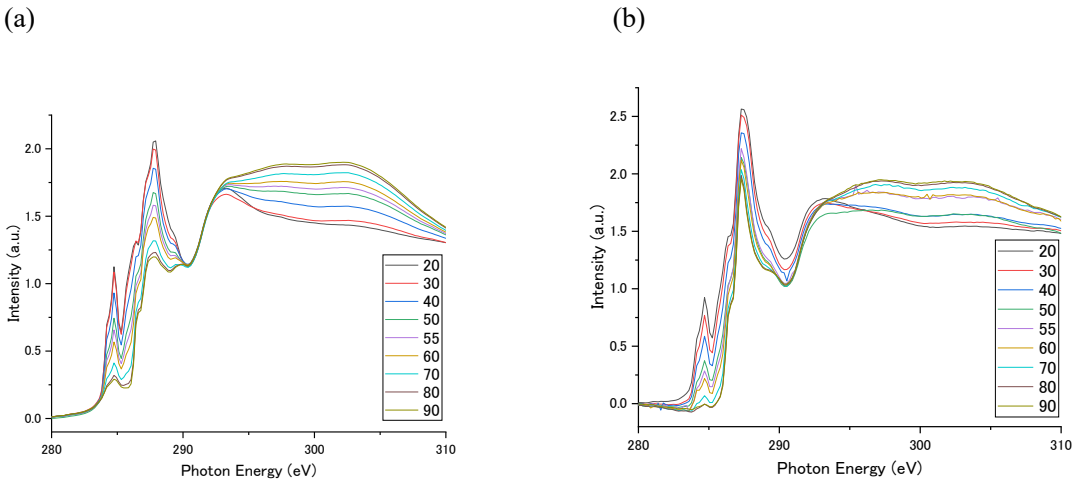

Figure 1. C 1s NEXAFS spectra of (a) pristine Y6 and (b) Y6 after 24 hours of thermal annealing.

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