Structure Control and Precise Characterization of Nanostructured Organic Heterojunction Photovoltaics by Synchrotron X-ray Structure Analyses

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Organic photovoltaic devices (OPVs) are attractive significant attention and regarded as the most promising technology for energy generation applications. The morphology control of the active layer in solar cells is of great importance in improving the device efficiencies. Since exciton dissociation occurs at the interface of the donor and acceptor materials, a large interfacial area should allow maximum exciton dissociation. In order to achieve high device performance, the domain sizes of the donor and the acceptor need to be optimized.

Recently, nano-imprint technique (NI) is being investigated as a method for producing optimized morphologies in OPVs with ordered bulk heterojunction (OHJ). NI is a simple, low cost and high-resolution surface patterning method. The molds with various types of surface morphology are mechanically pressed onto a polymer substrate, and then the nano-structures are transferred on the surfaces (Fig. 1.). The nano-imprinted OPVs show not only the formation of continuous phases with OHJ but also a significant degree of molecular alignment by the process of NI. In general, nano-structured OPVs have been produced by the NI of an organic donor, and then fullerene acceptor materials were subsequently deposited by spin cast from a selective solvent or evaporation. Here, it should be mentioned that these nano-imprinted structures located in not outermost surface but insides of devices, so called ‘buried’ structure (Fig. 2.). Furthermore, OPVs are usually annealed for the purpose of increasing performance due to the crystallization of organic donor and nano-scale phase separation state. So the understanding of molecular aggregation state of organic donor and OHJ are critical for the improvement of performances of OPVs. However, the nature of OHJ and the molecular aggregation states are still unclear, even for classical system as poly(3-hexylthiophene) (P3HT) and [6, 6’]-phenyl C61-butyric acid methyl ester (PCBM). P3HT exhibits high hole mobility and greate self-organization capacity, so P3HT act as an electron donor. On the other hand, PCBM works as an electron acceptor, because PCBM shows high electron mobility and good solubility for organic solvents.

In this study we evaluated the OHJ and molecular aggregation state of nano-structured OPVs. Nano-imprinted surface morphology was observed by atomic force microscopy (AFM). Also, ‘buried’ nano-structure and molecular aggregation state of P3HT were characterized by synchrotron radiation small angle X-ray scattering (SR-SAXS) and grazing incidence wide angle X-ray diffraction (GIXD) at the BL03XU beam line of SPring-8, respectively.