RECENT PROGRESS IN STRUCTURAL STUDY OF CRYSTALLINE POLYMERS BY UTILIZING QUANTUM-BEAM TECHNIQUES

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ABSTRACT

Recent development in structural study of crystalline polymers has been attained by remarkable progress in characterization techniques. For example, the combination of highly brilliant X-ray beam with highly-sensitive 2-dimensional detector has allowed us to perform the highly-time-resolved and highly-quantitative study of the structural evolution process in the phase transitions of crystalline polymers. (i) In particular the usage of synchrotron radiation (SPring-8 in Japan, for example) has lead us to the successful construction of the simultaneous measurement system of wide-angle X-ray diffraction (WAXD), small-angle X-ray scattering (SAXS), and vibrational spectroscopy (FTIR and Raman), as shown Figure. For example, the structural evolution in the isothermal crystallization process from the melt was revealed clearly from the wide hierarchical levels from molecular structure to spherulite. (ii) Another good example is about the stress-induced solid-state phase transition of oriented poly(tetramethylene terephthalate). The transmission-type FTIR data showed the chain conformational change between the α and β forms, where the α and β forms take the *gauche*- and *trans*-type conformations respectively. Information of packing structure change attendant with order-to-order phase transition was obtained by WAXD data. The SAXS data revealed a remarkable change in lamellar stacking structure *after* the completion of the phase transition in the crystal lattice for the first time. These information allowed us to interpret the molecular-level reason why this polymer is mechanically tough and utilized widely as an engineering plastic. (iii) Another progress is an accurate determination of hydrogen atomic positions in the crystal lattice. Information of hydrogen atomic positions in the crystal lattice is indispensable for the quantitative prediction of accurate ultimate physical properties of polymer crystals. However, because of the generally poor X-ray diffraction data, the extraction of hydrogen atomic positions is actually impossible. We utilized the wide-angle neutron diffraction (WAND) technique with brilliant neutron beam in J-PARC of JAEA, Tokai-mura. The positions of hydrogen atoms were successfully extracted for polyethylene, poly(vinyl alcohol) and so on as typical examples.

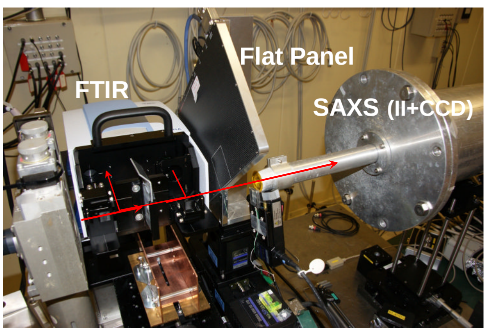

Figure 1. Simultaneous measurement system of WAXD/SAXS/FTIR data installed in SPring-8, Japan.