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|  MLF Experimental Report | 提出日 Date of Report April 24, 2015 |
| 課題番号 Project No. 2014PX0008 実験課題名 Title of experiment Clarification of Structure-Property Relationship in the Crystalline Phase Transitions of Polymers on the Basis of Wide-angle Neutron Diffraction Measurement as a Trial for the Construction of New Utilization Status of i-BIX System 実験責任者名 Name of principal investigator Kohji Tashiro 所属 Affiliation Department of Future Industry-Oriented Basic Science and Materials, Toyota Technological Institute | 装置責任者 Name of responsible person Katsuhiko Kusaka 装置名 Name of Instrument/(BL No.) i-BIX 実施日 Date of Experiment 2015年3月12日～3月19日 March 12, 2015 – March 19, 2015 |

試料、実験方法、利用の結果得られた主なデータ、考察、結論等を、記述して下さい。(適宜、図表添付のこと)
 Please report your samples, experimental method and results, discussion and conclusions. Please add figures and tables for better explanation.

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| 1. 試料 Name of sample(s) and chemical formula, or compositions including physical form. (1) Totally-deuterated high-density polyethylene $-(CD_2CD_2)_n-$ (2) Poly(vinyl alcohol)-iodine complex $-(CH_2CH(OH))_n- + KI_3$ |
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| 2. 実験方法及び結果 (実験がうまくいかなかった場合、その理由を記述してください。) Experimental method and results. If you failed to conduct experiment as planned, please describe reasons. <p>For the purpose of improving the quality of polymer materials it is necessary to clarify the structure-physical property from the molecular level. The crystal structure may be assumed as a ultimate state of the bulk samples, and the detailed analysis is needed including the clarification of the hydrogen atomic positions. In the present experiment, at first, the wide-angle neutron diffraction pattern of the highly-oriented totally-deuterated high-density polyethylene (DHDPE) sample has been measured again because the sensitivities and their homogeneity of the detectors of i-BIX system were revised. The result may be one of the most standard examples of the neutron structure analysis of the crystalline polymers.</p> <p>Another experiment performed in the present study was the measurement of the neutron diffraction patterns for poly(vinyl alcohol) (PVA)-iodine complex samples. This complex is well known as a polarizer, the crystal structure of which had been unsolved for a long time. We performed the X-ray crystal structure analysis of these PVA-iodine complexes as shown in Figure 1. The PVA chains and iodine chains are arrayed in parallel along the c axis. The unsettled problem in the X-ray structure analysis is the determination of the spatial positions of the PVA chains in the complex. This is because the X-ray scattering power of iodine ions is too strong compared with that of C and O atoms, making it difficult to determine the atomic positions of PVA chains uniquely. The cross-sectional-area of neutron scattering is almost</p> |
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2. 実験方法及び結果(つづき) Experimental method and results (continued)

comparable between iodine and carbon atoms, allowing us to determine the positions of these atoms more accurately than the X-ray analysis. The results should be an important trigger for the improvement of the polarizer from the industrial point of view. One example of the diffraction pattern obtained for PVA-iodine complex is shown in Figure 2, where the diffraction signals collected in one particular detector at the different timings were summed up together. The conversion of this type of diffraction data to the pattern of the reciprocal lattice system is now being made, which may give us the so-called fiber diffraction pattern of PVA-iodine complex sample, useful for the normal analysis process.

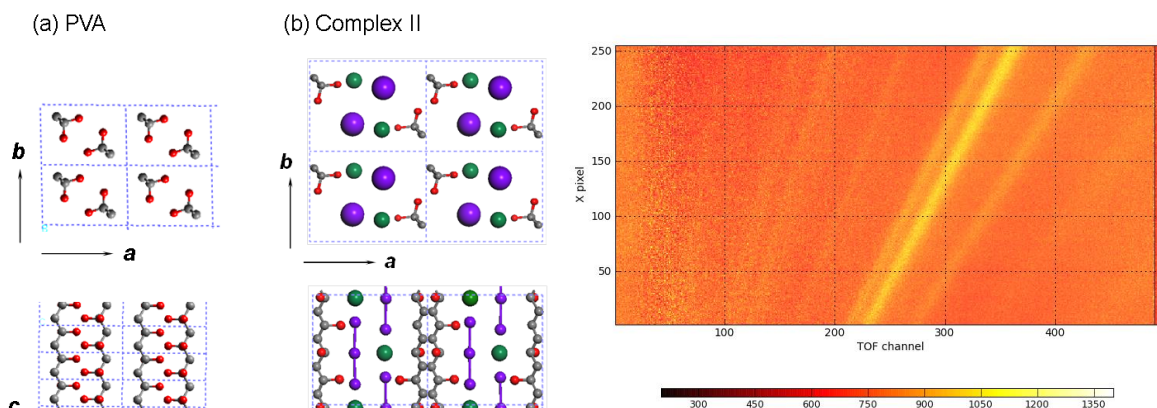


Figure 1 Crystal structure of (a) PVA and (b) PVA-iodine complex (Macromolecules, 48, 2138 (2015)).

Figure 2 Wide-angle neutron scattering pattern of PVA-iodine complex collected by a detector in the time-flight measurement.