

W0266

To Extract Hydrogen Atom Positions in Polymer Crystal: A Utilization of Wide-Angle Neutron Diffraction System with 2-Dimensional Imaging Plate Detector. Kohji Tashiro^{1*}, Ichiro Tanaka², Takashi Oohara³, Nobuo Niimura², Kazuo Kurihara³, Ryota Kuroki³, and Satoru Fujiwara³, ¹Department of Future Industry-Oriented Basic Science and Materials, Toyota Technological Inst., Tempaku, Nagoya 468-8511, Japan; ²Dept. of Technology, Ibaraki Univ., Hitachi, Ibaraki 316-8511, Japan; ³Advanced Science Research Center, Japan Atomic Energy Inst., Tokai-mura, Ibaraki 319-1195, Japan.

Extraction of hydrogen atom positions was made for fully-deuterated and hydrogenous samples of polyethylene, isotactic polypropylene, poly(vinyl alcohol) etc. on the basis of wide-angle neutron diffraction data collected with the 2-dimensional imaging plate detector. In the case of polyethylene, for example, the hydrogen atoms were clearly detected as positive (for deuterated sample) and negative (for hydrogenous sample) peaks in the neutron Fourier maps. The convergence of atomic coordinates in the least squares refinement was excellent. In the X-ray structure analysis the hydrogen atom positions had to be fixed in the refinement process. The electron diffraction, the data of which were collected for solution grown single crystals, gave the stereochemically unacceptable geometry because of multiple scattering effect.