MLF Experimental Report	提出日 Date of Report 2011/6/29
課題番号 Project No. 2010A0010 実験課題名 Title of experiment Single crystal neutron diffraction study of microcrystalline powder of biomolecules by pseudo-single crystal method 実験責任者名 Name of principal investigator Tsunehisa Kimura 所属 Affiliation Kyoto University	装置責任者 Name of responsible person Ichiro Tanaka, Katsuhiro Kusaka 装置名 Name of Instrument/（BL No.） BL-03 IBARAKI biological crystal diffractometer 実施日 Date of Experiment From 13:00 on the 12th of Nov. to 13:00 on the 13th of Nov., 2010.

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.

1. 試料 Name of sample(s) and chemical formula, or compositions including physical form.

Magnetically oriented microcrystal array (MOMA; a composite in which microcrystals are oriented three-dimensionally in a polymer matrix) of hen egg-white lysozyme, and of cellobiose were fabricated and subjected to the neutron diffraction measurements. Since a number of diffraction spots were observed previously in the case of an L-alanine MOMA without deuterium substitution of a matrix polymer, no attention was paid in this study to the deuterium substitution.

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.

Diffraction measurement was carried out for a lysozyme MOMA. Irradiation time was about 20 hours, and the irradiation beam wave length was 4.3-7.0Å. Accelerator power was 120kW, and 14 detectors were used for data collection. Histogram processing was performed for the obtained data and correction of detector sensitivity was carried out. No diffraction spots were observed.

Cellobiose of MOMA was also subjected to the diffraction measurement. Irradiation time was about 3 hours. The irradiation beam wave length was 4.3-7.0Å. Accelerator power was 120kW, and 14 detectors were used for data collection. Histogram processing was performed for the obtained data and sensitivity correction of detector was carried out. Diffraction spots of the (013), (130) and (123) planes were observed. Fig. 1 shows the diffraction patterns of the three different planes, that is, (013), (130) and (123) planes. Due to the orientation fluctuation of microcrystals in MOMA, diffraction spots exhibit larger spot size in comparison to the spots obtained using a real single crystal. Even without deuterium substitution for the matrix polymer,

2. 実験方法及び結果（つづき） Experimental method and results (continued)

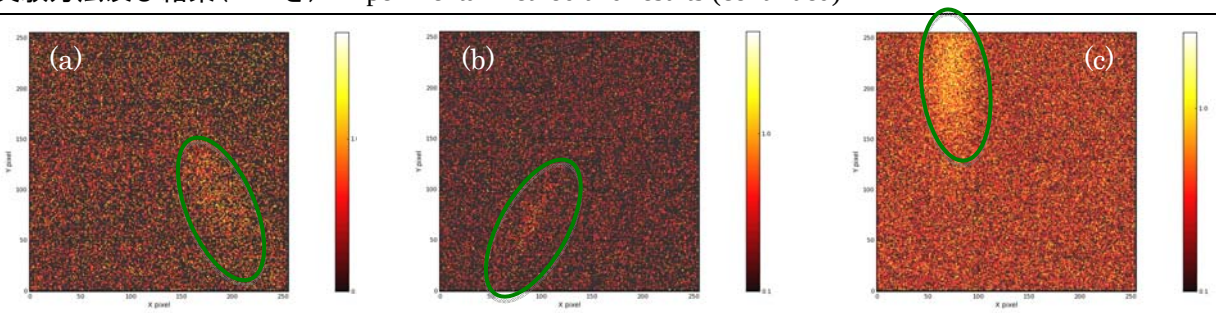

Figure 1. Neutron diffraction spots for the (013) (a), (130) (b), and (123) (c) planes obtained for the cellobiose MOMA.

We did not observe diffraction spots for the lysozyme MOMA probably because the diffraction intensity of proteins is weak compared with that from low molecular weight organic compounds such as cellobiose, being overwhelmed by background due to hydrogen atoms in a matrix polymer of the MOMA. We believe we will succeed in acquisition of diffraction spots by substitution of hydrogen atoms by deuterium.