MLF Experimental Report	提出日 Date of Report 10 Apr., 2016
課題番号 Project No. 2015PM0004 実験課題名 Title of experiment Correlation effects among thermal displacements of atoms by diffuse neutron scattering measurement 実験責任者名 Name of principal investigator Takashi Sakuma 所属 Affiliation Ibaraki University	装置責任者 Name of responsible person Toru Ishigaki 装置名 Name of Instrument/（BL No.） iMATERIA (BL-20) 実施日 Date of Experiment 7 Mar., 2016

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.

Silver Iodide （AgI） pressing pressure：0 MPa, 185 MPa, 370 MPa, 556 MPa
Copper Iodide （CuI） pressing pressure：0 MPa, 185 MPa,370 MPa, 556 MPa

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.

The AgI and CuI samples were prepared by a treatment of pressing pressure in rigid dies of diameter 5 ϕ . The applied pressure was changed in the range from 0 to 556 MPa. After the pressing, samples were crashed and reduced to powder by agate mortar for neutron diffraction measurement. These powder samples were sealed in V-Ni cylinder type container of diameter 6 ϕ . Neutron diffraction measurements were performed with iMATERIA installed at the MLF in J-PARC. All powder samples of AgI and CuI were measured under the room temperature. The diffraction intensities were collected by Time of Flight methods.

The observed powder diffraction intensities of AgI at 295 K are shown in Figure 1. It is seen that the peak positions and full-width at half-maximum (FWHM) of Bragg lines do not change significantly with the pressing pressure. Meanwhile, there is a drastic change of Bragg intensities with the increase of applied pressure near *tof* ~ 5-6 10^4 μs. It is well known that the stable phase of AgI at room temperature is the β-phase (wurtzite) and the γ-phase (zinc blende). Three Bragg lines near *tof* ~ 5-6 10^4 μs which are typical character in hexagonal crystal structure of the β-phase. The scattering intensity of three Bragg lines has a tendency to converge to the middle

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

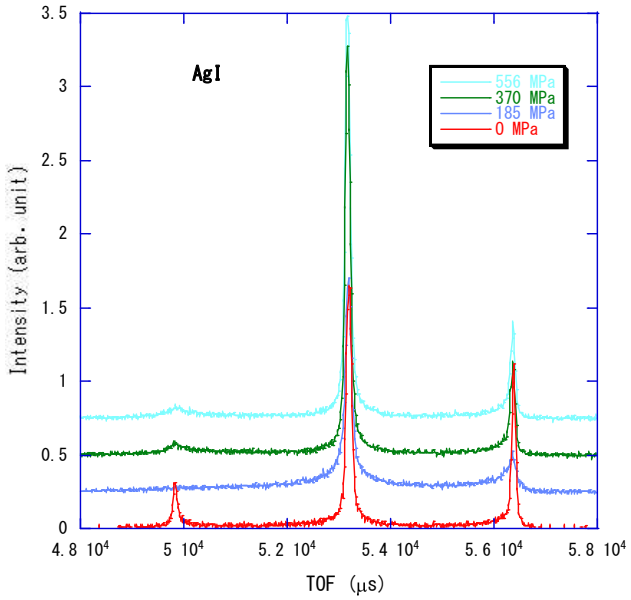

Figure 1. Scattering intensity of AgI.

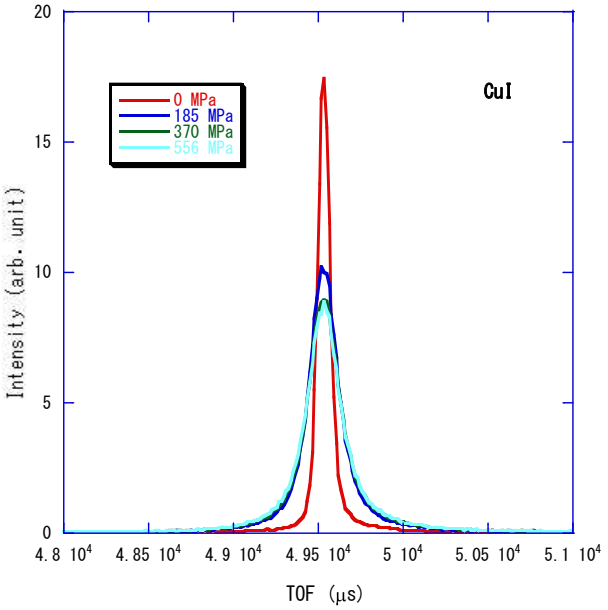

Figure 2. Scattering intensity of CuI.

Bragg line at high pressing pressure; which suggests that the crystal structure of the β-phase changes to the γ-phase by the increase of pressing pressure.

The observed powder diffraction intensities of CuI at 295 K are shown in Figure 2. The peak positions of Bragg lines do not change with pressing pressure. Meanwhile, there is a sudden increase in the FWHM of Bragg lines above 185 MPa. This result is similar to that of Ag_2O. In the case of Ag_2O, the value of FWHM increases linearly from 0 to 300 MPa, and it is almost constant above 300 MPa. A new crystal phase of Ag_2O occurs above 300 MPa. This would suggest that the crystal structure of CuI has a new phase above 185 MPa. The microstructural effects of TOF back-to-back exponentials type profile are represented with strain and size terms in Pseudo-Voigt functions [1]. We need to estimate these strain and size terms in CuI by the Rietveld method.

[1] Y. Ishikawa, T. Sakuma, H. Takahashi, S. A. Danilkin, Solid State Ionics 262(2014)622.