MLF Experimental Report	提出日 Date of Report June 24, 2013
課題番号 Project No. 2012B0234 実験課題名 Title of experiment Nuclear and magnetic structures in the spin-1/2 kagome lattice antiferromagnet $Cs_2Cu_3SnF_{12}$ 実験責任者名 Name of principal investigator Kittiwit Matan 所属 Affiliation Mahidol University	装置責任者 Name of responsible person Kittiwit Matan 装置名 Name of Instrument/（BL No.） BL-08 実施日 Date of Experiment March 11-15, 2013

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.

A power sample of $Cs_2Cu_3SnF_{12}$ is filled in a vanadium can with the diameter of 1 cm. The can is about 60% full.

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.

Time-of-flight powder neutron diffraction was performed on the distorted kagome lattice antiferromagnet $Cs_2Cu_3SnF_{12}$ to study its nuclear and magnetic structure at low temperatures. A powder sample is filled in a 1cm-diameter vanadium can and cooled to base temperature of 10 K using a closed cycle He-4 cryostat. The data are collected by three detector banks, which we will called LA (low-angle bank), QA (90-degree bank), and BS (back-scattering bank) with the highest resolution. The measurements were done at four temperatures, 10 K (below T_N = 20 K), 25 K, which is right above T_N, 150 K (below T_f = 185 K, where the structural phase transition occurs), and 200 K. The counting time at each temperature is about 30 hours. After the data reduction process and normalization, the reduced scattering intensity of each detector bank is plotted as a function of either time-of-flight or d-spacing.

At the base temperature of 10 K. we observe peak magnetic Bragg peaks on top of the fundamental nuclear Bragg peaks at **Q** = (2,0,2) and (2,2,0). We note that the peaks are indexed using an approximate structure, where the space group is R-3, and the lattice parameters are a = 14.21 and c = 20.18, since the true structure at low temperature of this material is not yet known. Figure 1 shows extra scattering intensity at 10 K compared to the data the 25 K at (2,0,2) and (2,2,0) for the LA, QA and BS detectors, indicative of the magnetic Bragg peaks.

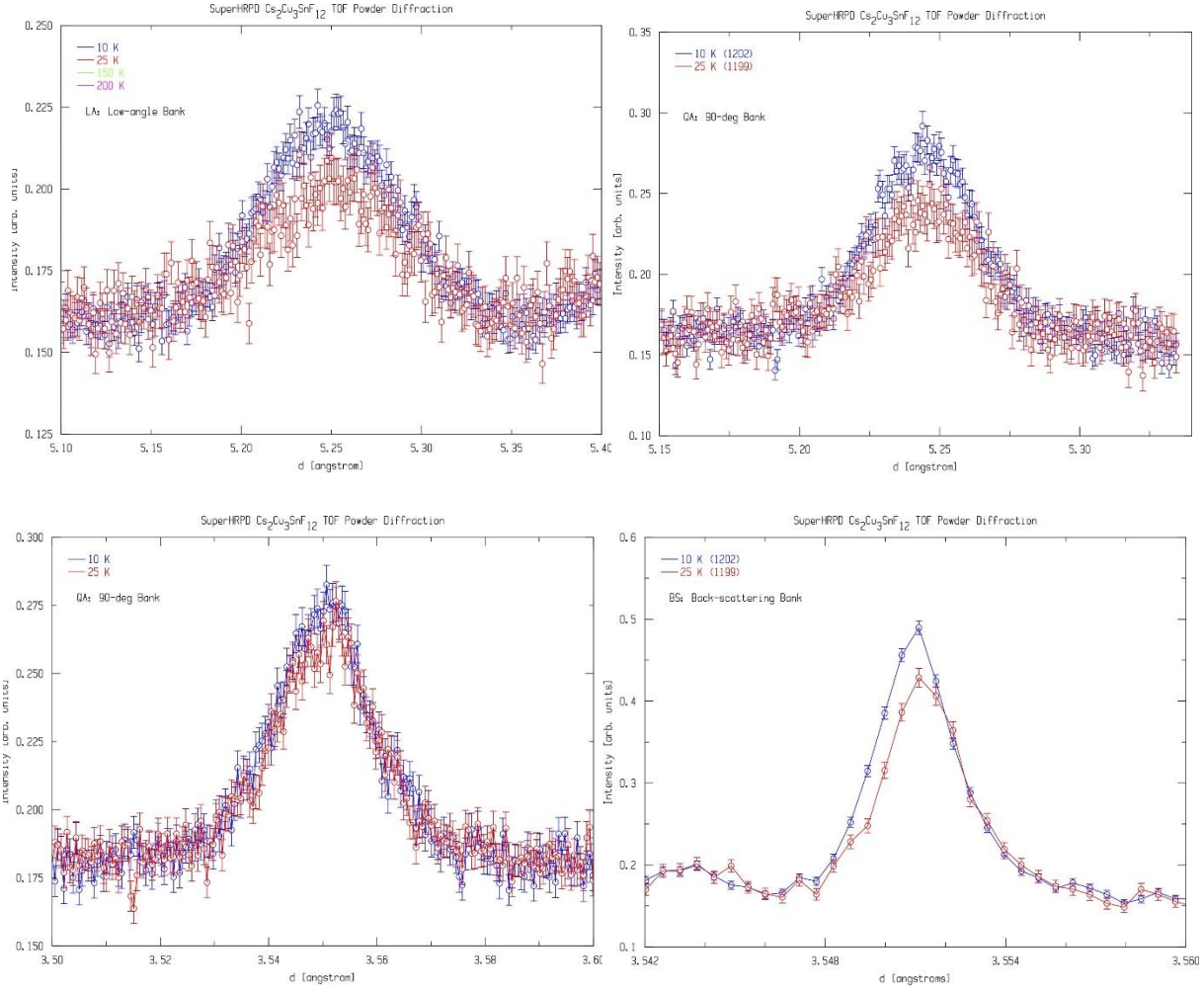

Figure 1. Top panels show the magnetic Bragg peak at (2,0,2) in the LA (left) and QA (right) detectors. Bottom panels show the magnetic Bragg peak at (2,2,0) in the QA (left) and BS (right) detectors.

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

At the structural phase transition, we observe the doubling of a unit cell, resulting in superlattice reflections. Figure 2 shows a group of superlattice peaks observed at 150 K but not at 200 K indexed by odd integers in H or/and K. These superlattice peaks are relatively small compared to the fundamental reflections; in the figure the fundamental reflections are (2,4,4) shown on the left and (0,0,9) shown on the right of the figure. In addition, we observe the splitting of the (2,4,4) peak suggesting that the true crystal structure is not exactly R-3. However, currently, the correct space group is unknown and further analysis is needed. We note that the splitting of some of the fundamental reflections can only observed using the high-resolution BS detector. The resolution of the LA and QA detectors is not enough to resolve the splitting and hence the data from those two sets of detectors can be refined using the spaces group R-3.

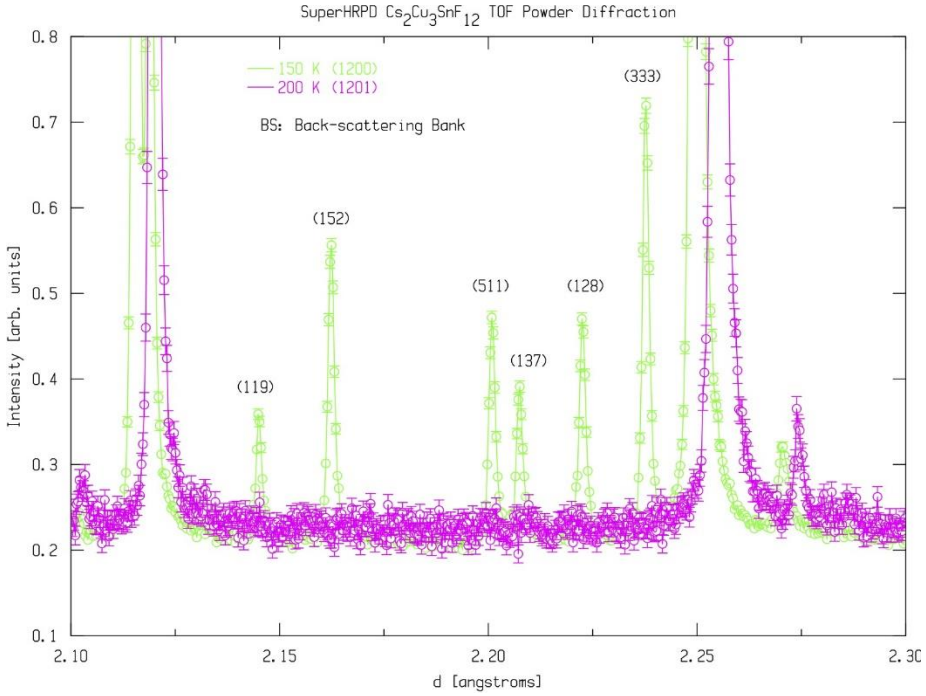

Figure 2. Superlattice reflections at odd integers in H or K between two fundamental reflections (2,4,4) at d = 2.112 angstroms, which splits into two peaks, and (0,0,9) at d = 2.112 angstroms, which does not split.

In summary, we performed high-resolution time-of-flight powder neutron diffraction on $Cs_2Cu_3SnF_{12}$ to study its nuclear and magnetic structure at low temperatures. We observe the magnetic Bragg peaks at 10 K, which disappears above T_N = 20 K. This magnetic peaks are very weak and lie on top of the structural peaks, making it difficult to detect. As the result, we can only observe two of such magnetic peaks. In addition, we observe the superlattice peaks, which are due to the structural transition at T_f = 185 K. These superlattice peaks are small compared to the fundamental peaks indicating of small lattice distortion. Furthermore, the splitting of some fundamental Bragg peaks with finite H and K is observed. The splitting is not observed at (0,0,L). This splitting of the fundamental peaks suggests that the symmetry of the crystal is not exactly R-3 as we have expected. We note that $Rb_2Cu_3SnF_{12}$, which is a closely related compound to $Cs_2Cu_3SnF_{12}$, crystallizes in R-3 at room temperature. This difference of the crystal structure could explain the observed difference in the magnetic ground states of these two compounds; while the ground state of $Rb_2Cu_3SnF_{12}$ is valence bond solid, S = ½ spins in $Cs_2Cu_3SnF_{12}$ order.