Study of the Magnetic Structure of Single Crystal $YBaCuFeO_5$ Using Inelastic Neutron and X-ray Scattering

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Abstract

Multiferroics has been an extensively studied subject because it plays as an important platform for studying the cross-coupling between the different degrees of freedom in the crystal space, such as spin, orbital, charge, and lattice. Using magnetization, dielectric constant on a high-quality single crystal $YBaCuFeO_5$(YBCFO) with the modified floating zone growth method, we demonstrate that the crystal shows two antiferromagnetic transitions at $T_{N1} \sim 455$ K and $T_{N2} \sim 175$ K. At T_{N2}, the commensurate spin ordering transforms to a spiral magnetic structure with a propagation vector of $(h/2\ \ k/2\ \ l/2\pm\delta)$, where h, k, and l are odd, and the incommensurability δ is temperature dependent. In order to understand the dynamic behavior of the spiral magnetic ordering, we applied inelastic neutron scattering to study the spin ordering of the crystal YBCFO on the beamlines SIKA and PELICAN of ANSTO. On PELICAN, we focused on two-phase regimes, commensurate (T = 250 K) and incommensurate (T = 110 K), and observed both phases showing a very steep excitation behavior which could extend up to 5 meV. In addition, there are excitation signals between the magnetic peak have the same behavior as the magnetic one. So as to know in details of the dynamics behavior of the spiral magnetic ordering of YBCFO, we will study its electronic and magnetic structure through elastic and inelastic X-ray scattering.

Keywords – Double Perovskite Structure, Magnon, INS

Introduction

Perovskites ABO_3 plays an important role in the application and research of condensed matter physics and novel functional materials, such as high-temperature superconductors, ferroelectrics, magnetic reluctance, multiferroic, thermoelectric, etc. This study will focus on the double perovskite iron-based oxide $YBaCuFeO_5$(YBCFO), which is reported to have multiferroic properties. In order to study the anisotropy of YBCFO, single crystal samples were grown with the floating zone method. Through the neutron scattering experiment, the magnetic structure of the commensurate phase is q = $(h/2\ k/2\ l/2)$ at room temperature. When the temperature is lower than T_{N2}, the magnetic structure changes to the incommensurate phase with a propagation vector q = $(h/2\ \ k/2\ \ l/2\pm\delta)$, δ increases with decreasing temperature. The dynamic behavior of the spin-wave generated by the spiral magnetic structure and the coupling relationship with the crystal lattice will also be in interest. Also the interaction between Fe^{3+} / Cu^{2+} is greatly affected. The contribution of Fe^{3+} / Cu^{2+} in the magnetic structure will be the focus on.

Experiments

In order to understand the magnetic structure, using inelastic neutron scattering is a useful method which helps to explore dynamic behavior, because neutrons are very sensitive to magnetic structures. The research is mainly carried out on the beamline SIKA and PELICAN of ANSTO, Australian, and the energy is focused on low energy (< 5 meV). The high-quality single-crystal sample was fixed on the aluminum holder. The excitation behavior of the magnetic structure in the reciprocal space to the energy transfer was measured, as well as the coupling between the magnon and the temperature was observed. A higher energy measurement was then performed (6 ~ 15 meV) at TAIPAN. In order to understand the behavior of higher energy and to distinguish the contribution of Fe/Cu, inelastic X-ray scattering experiments were also performed in Spring-8, Japan.

Results

Inelastic Neutron Scattering

Frist, we focus on low energy at magnetic structure behavior, the temperature in Fig. 1. is lower than T_{N2} is incommensurate structure. It is a reasonable result with two reflection peaks because of the magnetic structure mentioned above. But the intensity of the reflection in inelastic scattering is increase as the temperature increases.

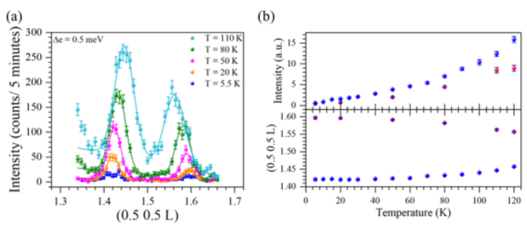

Fig. 1. Temperature dependent (a) energy-fixed (energy transfer = 0.5 meV) q-scan at q = (0.5 0.5 L). (b) The

evolution of the integrated intensity and q-vector as a function of temperature of (a).

The experiment was done on beamline PELICAN which station is the Time of Fly experimental station. As shown in Fig. 2., the diffraction peak below the TN2 magnetic structure splits into two, the same behaver in Fig. 1, also intensity is weakened at the low temperature. However, there is a signal at L = 0.5 ~ 1.5 also, and increases with temperature, and L < 0.5 and L > 1.5 have no similar signals.

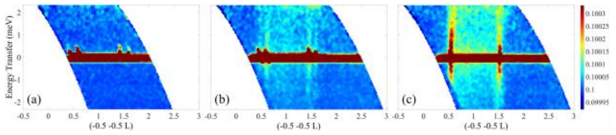

Fig. 2. Time of fly spectra at (a) 1.5 K, (b) 110 K, (c) 250 K. It is clear to see the sharp dispersions from the commensurate and incommensurate magnetic phases.

Inelastic X-ray Scattering

The above results are all focused on low energy. In this part of the experiment, the excitation energy is increased to 6 meV. As shown in Fig. 3., the inelastic scattering signal increases with temperature, which is consistent with the low energy behavior and also the middle part. The region is fitted, and its integrated intensity also has this behavior. It can be inferred that the magnetic structure of the sample has a coupling behavior with the intermediate region.

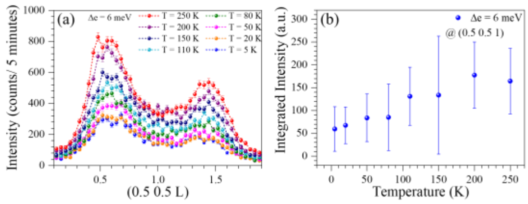

Fig. 3. Temperature dependent energy-fixed (energy transfer = 6 meV) q-scan at q = (0.5 0.5 L). (g) Temperature dependent curve of integrated intensity of middle peak. (h) Magnetic structure dispersion behavior at 250 K.

This part of the experiment was carried out on the Spring-8 beamline BL12XU. The result of normal temperature has been obtained. The incident energy is focused near the Fe K-edge, the energy loss is about 8 eV with excitation signal. It can be inferred that the system generates a collective excitation, the energy loss is greater than 20 eV is K_{β}.

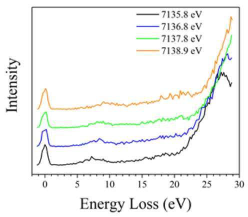

Fig. 4. Inelastic X-ray scattering spectrum at different incident light energy.

Discussion

From the experimental results mentioned in the previous paragraph, the magnetic behavior of YBCFO is very special and complex. Inelastic signals decrease with increasing temperature and are quite different from general elastic results of magnetic. Also, the reflection peak in the middle region has the same behavior. It is not known whether the signal comes from magnetics or not, and the relationship with Fe^{3+} / Cu^{2+} will be one of the focuses of future research. In inelastic X-ray part, we will also be understood through q-space analysis and discussed with the neutron inelastic scattering results. For the relationship between inelastic signals and temperature, it is speculated that magnon couples with phonon.

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