1B, 4C, 16A2/2004G244

Orbital Ordering and the dilute effect in copper fluoride

Youichi MURAKAMI*[1,2], Naka TATAMI[1], Hidekazu TAMURA[1], Hironori NAKAO[1], Takeshi MATSUMURA[1], Yusuke WAKABAYASHI[3], Hiroshi SAWA[3], Shinichi ITO[4]
[1]Department of Physics, Tohoku University, Sendai 980-8578, Japan
[2]Synchrotron Radiation Research Center, JAERI, Sayo, 679-5148, Japan
[3]KEK-PF, Tsukuba, Ibaraki 305-0801, Japan
[4]KEK-KENS, Tsukuba, Ibaraki 305-0801, Japan

Introduction

It is well kown that charge-, spin-, and orbital orderings play important roles in strongly correlated electron systems. The long-range orderings have successfully observed by resonant x-ray scattering (RXS) and neutron scattering and so on. Impurity effect in the ordered states has raised interesting results; for example, in high Tc cuprates a small amount of impurity destroys the superconductivity and revive the magnetic order. The impurity effect in localied spin systems has also been intensively studied in the past 30 years. On the other hand, few studies on the effect are reported in orbitally odered systems. We have investigated the effect on a typical orbital ordering system $KCuF_3$ by substituting Zn for Cu. In this case we call the effect as the dilute effect because Zn ion has a closed shell ($3d^{10}$).

Experimental Results

Powder Diffraction and Resonant X-ray Scattering

High quality single crystals were grown using Bridgman method. Powder samples with uniform concentraiton were prepared by crushing the single crystals. Powder diffraction experiments were carried out at BL-1B using the imaging plate. The RXS experiments at Cu K absorption edge energy have been done at BL-4C and BL-16A2 with four circle diffractometer.

Figure 1 shows the lattice constants *a, c*, measured by powder diffraction experiments, as a function of Cu concentration at room temperature. Increasing Zn ions we found the difference between *a* and *c* become small and zero around x = 0.6. This result indicates that a structural phase transition from tetragnal to cuic occurs near this concentration. It is supposed Jahn-Teller distortion due to the orbital ordering in high Cu concentration releases with decreasing Cu concentration. To confirm this we have applied the RXS technique to this system. The RXS intensity corresponds to the order parameter of the orbital ordering through Jahn-Teller effect. The RXS intensities rapidly decrease with decreasing Cu ions and disappear around x = 0.6 at room temperature as shown in the inset of Fig. 1. Therefore, it is elucidated that the tetragonal and cubic phases are an orbital ordered and disordered phases, respectively.

We have made concentration-temparature phase diagram from the powder diffraction data measured in high and low temperature regions using furnace and cryostat. The phase diagram is shown in Fig. 2. The ordering temperature decreases with decreasing Cu ions and disappears at x = 0.55 in the extrapolation to T = 0 K. This concentration is much larger than that of the conventional dilute mangets: the arrow in Fig. 2 shows the concentration of order-disorder threshold in a 3 dimensional magnet of simple cubic. This result is attributed to the orbital modulation around the Zn site; the modulation may expand to several unit cells for one Zn ion.

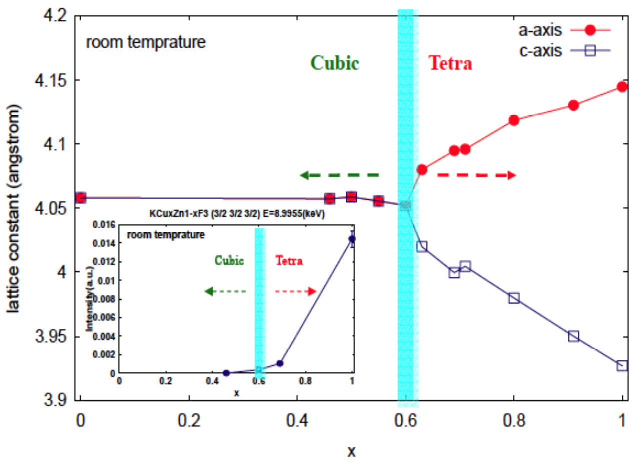

Figure 1. Lattice constants *a, c* at room temperature as a function of Cu concentration. Inset: Concentration dependence of RXS intensities.

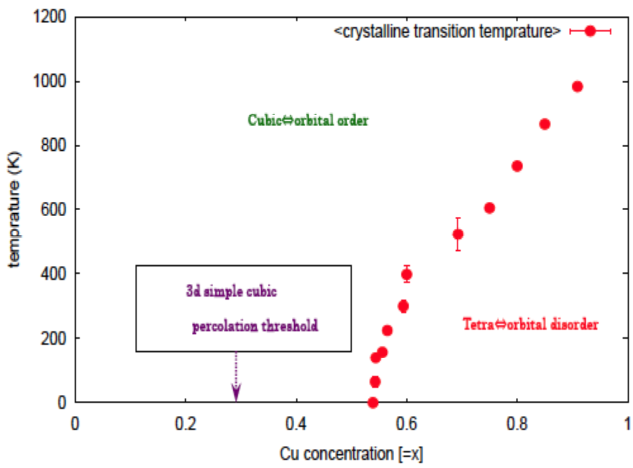

Figure 2. Cu concentration vs. temprature phase diagram.

* murakami@iiyo.phys.tohoku.ac.jp