Materials Science

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Structural studies on metal-insulator transition in $K_2Cr_8O_{16}$

Masahiko ISOBE*[1], Kunihiro HASEGAWA[1], Akiko NAKAO[2], Hironori NAKAO[2], Yutaka UEDA[1]
[1]ISSP, The Univ. of Tokyo, Kashiwa, Chiba 277-8581, Japan
[2]KEK-PF, Tsukuba, Ibaraki 305-0801, Japan

Introduction

Recently, we have investigated a rare mixed-valent chromium oxide $K_2Cr_8O_{16}$ [1]. The hollandite $K_2Cr_8O_{16}$ shows metallic conductivity, ferromagnetic order at 180 K, and a metal-insulator transition at T_{MI} = 95 K. This compound is quite unique in the aspect that it has a metal-to-insulator transition in a ferromagnetic state, and the resulting low temperature phase is a rare case of a ferromagnetic insulator. Any structural transition at the metal-insulator transition was expected. Then we checked any structural change below T_{MI} by laboratory x-ray diffraction. However, neither splitting of the diffraction peak nor additional peak has been observed. The patterns can be indexed by tetragonal I4/m symmetry in the whole temperature range measured (10-300K). In general, super-lattice reflections are too weak to be observed by laboratory x-ray diffraction. Therefore we aim to find any peak splitting and/or super-lattice reflections by synchrotron X-ray diffraction.

Experiments

We prepared polycrystalline of $K_2Cr_8O_{16}$ by a solid state reaction of a mixture of $K_2Cr_2O_7$ and Cr_2O_3 under 6.7GPa at 1273K for 1h. Single crystals were obtained using $K_2Cr_2O_7$ as self-flux under high pressure. Synchrotron x-ray diffractions were collected on a Rigaku imaging plate system by using Si-double-crystal monochromatized radiation at the beam line BL-8A.

Results and Discussion

We could not observe any splitting of diffraction peaks below T_{MI}. However, extra reflections with modulation wave vector q = (*h*/2, *k*/2, 0) were observed below T_{MI}. They are marked by arrows in Fig. 1. This indicates a super-lattice of √2 x √2 x 1 for the insulator phase. Figure 2 shows the temperature dependence of the intensity of super-lattice reflections. They gradually decrease in the intensity with increasing temperature and disappear around 100K corresponding to the metal-insulator transition. This means a second order structural transition to a lower symmetry from tetragonal I4/m below T_{MI}. The structural analyses below T_{MI} are now in progress.

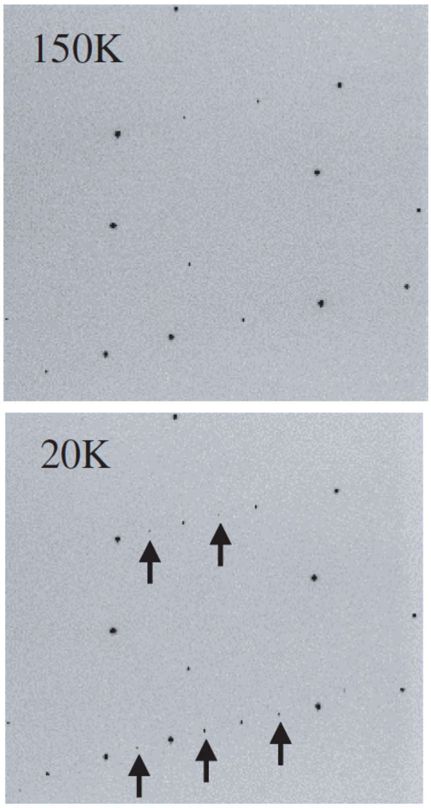

Fig. 1. Synchrotron x-ray diffraction photographs at 20 K and 150 K. At 20K, a series of super-lattice reflections with modulation wave vector q = (*h*/2, *k*/2, 0) are clearly observed, as indicated by arrows.

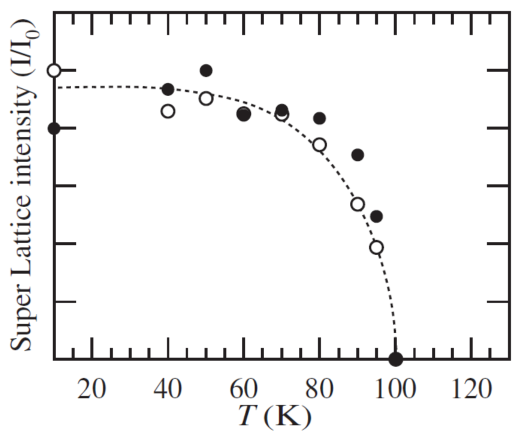

Fig. 2. Temperature dependences of the intensity of two super-lattice reflections.

Reference

[1] K. Hasegawa *et al.*, Phys. Rev. Lett. **103** (2009) 146403.

* isobe@issp.u-tokyo.ac.jp