Determination of Hole Distribution for $Sr_{14-x}Ca_xCu_{24}O_{41}$ Compound Using Cu XAS Measurement

Meng-Jie Huang (黃孟傑)[1], Hong-Ji Lin (林宏基)[1], Zhiwei Hu (胡志偉)[2], Chang-Yang Kuo (郭昌洋)[1], Fang-Cheng Chou (周方正)[1,3], and Chien-Te Chen (陳建德)[1]

[1]National Synchrotron Radiation Research Center, Hsinchu, Taiwan
[2]Max Planck Institute fur Chemische Physik Fester Stoffe, Dresden, Germany
[3]Center of Condensed Matter Sciences, National Taiwan University, Taipei, Taiwan

Corner-shared ladder $Sr_{14-x}Ca_xCu_{24}O_{41}$ compound is attracting so much research interest because it is the first superconducting copper-oxide material with a non-square-lattice layered arrangement. Determining of the hole distribution between edge-shared chain and corner-shared ladder is necessary for understanding of the mechanism of superconductivity in $Sr_{14-x}Ca_xCu_{24}O_{41}$ compound. There have been many attempts to determine the hole distribution. However, several researchers have reached different conclusions on this question. One is that holes stay mainly in the edge-shared chain despite the Ca substitution and the other is that considerable number of hole move to corner-shared ladder from the edge-shared chain upon Ca substitution. The major problem with those previous studies are that they do not observe the hole distribution using the most direct Cu X-ray absorption spectrum. Since the Cu X-ray absorption spectrum is the key to solve the hole distribution problem for $Sr_{14-x}Ca_xCu_{24}O_{41}$ ladder compound, we re-measurement and reanalyze the hole distribution in $Sr_{14-x}Ca_xCu_{24}O_{41}$ compound using the Cu X-ray absorption spectrum to answer this puzzling question. In Cu spectrum, we have interest in the energy range of 927-936eV (This is Cu L_3 absorption edge). Figure 1 depicts the result of this range in **E**//**a**,**c**. To obtain the more reliable data, we cleave the sample *in situ* to perform the measurement in total electron yield mode. The spectrum of this range consist of two different features located at 932.5eV and 934eV. The major configuration involved in the X-ray absorption for these two peak are $3d^9 \rightarrow 2p^5 3d^{10}$ (Cu^{2+} peak) and $3d^9\underline{L} \rightarrow 2p^5 3d^{10}\underline{L}$ (Cu^{3+} peak), respectively.

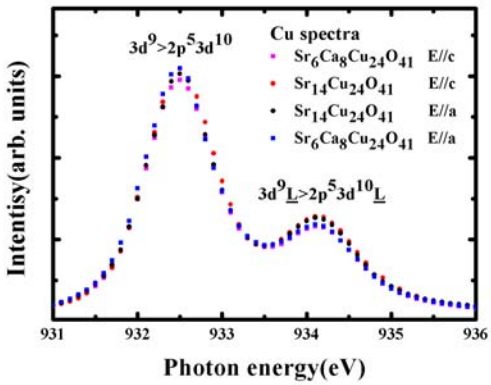

Fig. 1: Cu $2p_{3/2}$ XAS of $Sr_{14}Cu_{24}O_{41}$ sample and heavy-Ca doped $Sr_6Ca_8Cu_{24}O_{41}$ sample.

Previous works [1,2] are shown that even both the edge-shared chain and corner-shared ladder with same formal valence of Cu, the spectrum property of edge-shared chain and corner-shared ladder is very distinct. The difference of spectrum between edge-share chain and corner-shared ladder appears in Fig. 2. This diagram tells us that the higher-energy peak (Cu^{3+} peak) turn to be a very weak shoulder when the hole doped on the corner-shared ladder. In other words, if the holes all staid in the corner-shared ladder, the higher-energy peak (Cu^{3+} peak) should not be observed. In fact, it is evident that a considerable Cu^{3+} peak can be observed even under the heavy-Ca doped $Sr_{14-x}Ca_xCu_{24}O_{41}$ sample. Therefore, these data lead to the conclusion that the hole reside mainly in the edge-shared chain despite the Ca substitution.

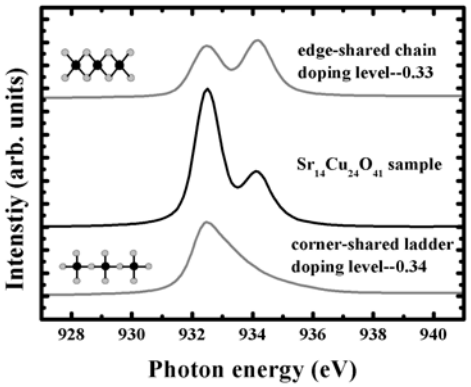

Fig. 2: The difference of spectrum between edge-shared chain and corner-shared ladder.

To be brief, this study investigates the hole distribution using Cu X-ray absorption spectrum. Using of the most direct Cu spectrum can be distinguished the edge-shared chain and corner-shared ladder components of spectrum to give a conclusive answer to the controversial question. The most holes reside in the edge-shared chain (about 5.3 holes) for $Sr_{14}Cu_{24}O_{41}$ sample and transferring about 0.3 holes to corner-shared ladder for $Sr_6Ca_8Cu_{24}O_{41}$ sample. We assure this finding is of great importance for understanding of superconductivity of corner-shared ladder $Sr_{14-x}Ca_xCu_{24}O_{41}$ compound.

References

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