Hole distribution in the underdoped, optimally doped, and overdoped superconductors (Tl0.5Pb0.5)Sr2(Ca1-xYx)Cu2O7

R. S. Liu*, J. M. Chenb and W. Y. Liangc

*Department of Chemistry, National Taiwan University, Taipei, Taiwan.
*bSynchrotron Radiation Research Center (SRRC), Hsinchu, Taiwan.
cIRG in Superconductivity, University of Cambridge, U.K.

We report high-resolution O K-edge X-ray-absorption near-edge-structure (XANES) spectra for the series of underdoped, optimally doped, and overdoped (Tl0.5Pb0.5)Sr2(Ca1-xYx)Cu2O7 compounds (x = 0 - 0.9) obtained using a bulk-sensitive total-fluorescence-yield technique. Near the O 1s edge, a well-pronounced pre-edge peak with maxima at ~ 528.3 eV is observed which is ascribed to excitations of O 1s electrons to O 2p holes located in the CuO2 planes. The intensity of the pre-edge peak increases linearly with the Ca doping over the entire range from the underdoped, through the optimally doped, to the overdoped region. This indicates that the effect of chemical substitution of Ca2+ for Y3+ is to induce hole states in the CuO2 planes near the Fermi level, which are important to control the Tc for the series of (Tl0.5Pb0.5)Sr2(Ca1-xYx)Cu2O7 compounds.

I. INTRODUCTION

It has been experimentally demonstrated that holes are responsible for superconductivity from the correlation between the superconducting transition temperature (Tc) and the hole concentration. [1] A precise knowledge of the unoccupied electronic structure near the Fermi level of these compounds is therefore an important first step toward comprehensive understanding the electronic states of holes and the mechanism of superconductivity. For this reason, direct experimental information on the electronic structures of these compounds is of particular importance.

The Tl-based septenary cuprate (Tl0.5Pb0.5)Sr2(Ca1-xYx)Cu2O7 (hereafter referred to as Tl-1212) has the highest Tc among the thallium cuprate systems with the so-called 1212 structure. The crystal structure of the Tl-1212 phase (Tl0.5Pb0.5)Sr2(Ca1-xYx)Cu2O7 can be described in terms of an intergrowth of double rock-salt-type layers [{Tl(Pb)}O]0(SrO) with double [Sr(Ca,Y)Cu2O4] oxygen deficient perovskite layers [2], formed by sheets of corner-sharing CuO5 pyramids interleaved with calcium and/or yttrium ions as shown in Fig. 1. This system exhibits superconductivity over the homogeneity range x = 0 ~ 0.5, with the superconducting transition temperature showing a maximum of 108 K at x = 0.2. [2] However, towards the high end of the Ca doping, the Tc of these compounds decreases which leads to a dome-shaped curve. Across the homogeneity range x = 0.6 ~ 1.0, the material also undergoes a metal-insulator transition at temperature above Tc.

![Figure 1](image-url)
Here, we report soft-X-ray-absorption measurements at the O K-edge in the series of (Tl_{0.5}Pb_{0.5})Sr_2(Ca_{1-x}Y_x)Cu_2O_7 samples using a bulk-sensitive fluorescence-yield-detection method.

2. EXPERIMENTAL

Samples with nominal compositions of (Tl_{0.5}Pb_{0.5})Sr_2(Ca_{1-x}Y_x)Cu_2O_7 were prepared by solid-state reaction method which has been reported in detail elsewhere [2]. The XANES measurements were carried out on the 6 m high-energy spherical grating monochromator (HSGM) beamline of the Synchrotron Radiation Research Center (SRRC) in Taiwan. [3]

3. RESULTS AND DISCUSSION

In Fig. 2 high-resolution O K-edge X-ray-absorption near-edge structure (XANES) spectra for the series of (Tl_{0.5}Pb_{0.5})Sr_2(Ca_{1-x}Y_x)Cu_2O_7 samples in the energy range of 526 - 540 eV were shown by measuring the total X-ray-fluorescence yield. As the Ca doping increases, this gives rise to a new pre-edge feature at ~ 528.3 eV for x ≤ 0.5. In addition, this pre-edge peak for x = 0 in Fig. 2 shifts by 0.1-0.2 eV to higher energies as the increase of the Y content. This indicates that the effect of chemical substitution of Ca^{2+} for Y^{3+} is to induce hole states with the O 2p character near the Fermi level. In analogy to results from other p-type cuprate superconductors [4], the pre-edge peak at ~528.3 eV in Fig. 2 for the series of (Tl_{0.5}Pb_{0.5})Sr_2(Ca_{1-x}Y_x)Cu_2O_7 samples can be ascribed to the excitations of O 1s electrons to O 2p holes located in the CuO_2 planes.

The intensity of this pre-edge peak increases linearly with the Ca doping for 0 ≤ x ≤ 0.5. This indicates that the effect of chemical substitution of Ca^{2+} for Y^{3+} is to induce hole states in the CuO_2 planes near the Fermi level. The intensity of this pre-edge peak closely correlates with the compositional variation of superconducting transition temperature, showing that holes generated in the O 2p orbitals within the CuO_2 planes play an important role to control the T_c of the titled system.

![Figure 2. O K-edge X-ray-absorption near-edge-structure spectra for the series of (Tl_{0.5}Pb_{0.5})Sr_2(Ca_{1-x}Y_x)Cu_2O_7 compounds with x = 0, 0.1, 0.2, 0.3, 0.4, 0.5, and 0.9 by measuring the total-X-ray-fluorescence yield. These spectra have been normalized to have the same height at the main peak of 537 eV.](image)

ACKNOWLEDGEMENTS

This research is financially supported by National Science Council of the Republic of China under the Grants NSC-86-2113-M-002-020 and NSC-86-2613-M-213-010

REFERENCES