Hole distribution in $Y_xPr_{1-x}Ba_2Cu_4O_8$ and $Y_xPr_{1-x}Ba_2Cu_3O_7$ probed by X-ray absorption spectroscopy

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Abstract

Utilizing high-resolution O K-edge X-ray absorption spectra, we report a comparative study on the variation of hole states with Pr doping for $Y_xPr_{1-x}Ba_2Cu_4O_8$ and $Y_xPr_{1-x}Ba_2Cu_3O_7$. The depletion rate of hole carriers in the CuO$_2$ planes with Pr doping in $Y_xPr_{1-x}Ba_2Cu_4O_8$ is considerably slower than that in $Y_xPr_{1-x}Ba_2Cu_3O_7$. The oxygen content affects the depletion rate of hole carriers in cuprates with Pr doping.

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Keywords: X-ray absorption spectra; Hole carriers

Pr substitution in $YBa_2Cu_3O_7$ has been a topic of extensive study. The absence of superconductivity and the anomalously high Neel temperature of 17 K of PrBa$_2$Cu$_3$O$_7$ (Pr123) have long remained controversial puzzles [1,2]. For $Y_xPr_{1-x}Ba_2Cu_3O_7$, $T_c$ decreases monotonically with increasing Pr doping level from $T_c = 80$ K for $x = 1$ to $T_c = 6$ K for $x = 0.3$ [3]. The critical Pr concentration required to quench superconductivity in $Y_xPr_{1-x}Ba_2Cu_3O_7$ is estimated to be $\sim 0.72$, which is larger than that of $\sim 0.55$ in $Y_xPr_{1-x}Ba_2Cu_3O_7$. Utilizing high-resolution O K-edge X-ray absorption spectra, we report a comparative study on the variation of hole carriers with Pr doping for $Y_xPr_{1-x}Ba_2Cu_3O_7$ ($x = 0$–1) thin films and polycrystalline $Y_xPr_{1-x}Ba_2Cu_3O_7$ ($x = 0$–1) samples.

X-ray absorption measurements were performed at the Synchrotron Radiation Research Center (SRRC) in Taiwan. The X-ray-fluorescence-yield absorption spectra were corrected for the energy-dependent incident photon intensity as well as for the self-absorption effects and normalized to tabulated standard absorption cross section in the energy range from 600 to 620 eV.

In Fig. 1(a), polarized O K-edge X-ray absorption spectra of the $Y_xPr_{1-x}Ba_2Cu_3O_7$ ($x = 0$–1) thin films for $E||ab$ polarization are reproduced. For $YBa_2Cu_3O_7$, the absorption feature at $\sim 528.4$ eV is ascribed to hole states in the CuO$_2$ planes (i.e., the Zhang-Rice (ZR) states), while the shoulder at $\sim 527.8$ eV corresponds to unoccupied states in the CuO chains. The absorption peak at $\sim 529.5$ eV is attributed to the upper Hubbard band (UHB). As noted from Fig. 1, upon Pr substitution, the spectral weight of the ZR states is strongly reduced, but the UHB intensity is significantly enhanced at the same time. This change is attributed to the well-known transfer of spectral weight from the ZR states to the UHB due to strong correlation effects in the CuO$_2$ planes.

Many models were proposed to explain the superconductivity suppression in PrBa$_2$Cu$_3$O$_7$ and related Pr-doped cuprates. The existence of Pr 4f($\zeta^2-\zeta^2$)-O 2p$_\pi$ hybridized states proposed by Fehrenbacher and Rice (FR) is widely considered to be one of the most promising models [2,4]. The FR model proposed that hole depletion in the CuO$_2$ planes with Pr doping is due to transfer of hole carriers from the CuO$_2$ planes into the...
Pr 4f–O 2p hybridized states or FR states. Fig. 1(b) presents the O K-edge X-ray absorption spectra of the Y$_x$Pr$_{1-x}$Ba$_2$Cu$_3$O$_7$ ($x = 0$–1) thin films for (a) $E||ab$ and (b)$E||c$ polarization. For comparison, the absorption spectrum of Pr123 is plotted as a dashed curve. The additional FR band is observed, as indicated by hatched lines.

In Fig. 2(a), the O K-edge X-ray absorption spectra of the polycrystalline Y$_x$Pr$_{1-x}$Ba$_2$Cu$_4$O$_8$ ($x = 0$–1) samples are presented. The pre-edge peak at $\sim$527.8 eV corresponds to excitations of the O 1s electrons to the O 2p hole states in the apical oxygen sites. The pre-edge peaks at $\sim$528.5 eV are due to the superposition of the O 2p hole states in the CuO$_2$ planes and CuO chains [6]. The absorption peak at $\sim$529.6 eV is ascribed to the upper Hubbard Cu 3d conduction band. As noted from Fig. 2(a), the pre-edge peaks at $\sim$528.5 eV originating from the O 2p hole states in the CuO$_2$ layers and CuO chains show a slight decrease in spectral weight with increasing the dopant concentration of Pr.