

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 $Y_xPr_{1-x}Ba_2Cu_3O_7$ and $Y_xPr_{1-x}Ba_2Cu_4O_8$. 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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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 $PrBa_2Cu_3O_7$ (Pr123) have long remained controversial puzzles [1,2]. For $Y_xPr_{1-x}Ba_2Cu_4O_8$, 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 $Y_xPr_{1-x}Ba_2Cu_4O_8$ is estimated to be ~ 0.72 , which is larger than that of ~ 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 $Y_xPr_{1-x}Ba_2Cu_4O_8$ ($x = 0-1$) 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 ~ 528.4 eV is ascribed to hole states in the CuO_2 planes (i.e., the Zhang-Rice (ZR) states), while the shoulder at ~ 527.8 eV corresponds to unoccupied states in the CuO chains. The absorption peak at ~ 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 $PrBa_2Cu_3O_7$ and related Pr-doped cuprates. The existence of Pr $4f_{(x^2-y^2)}-O 2p_\pi$ 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

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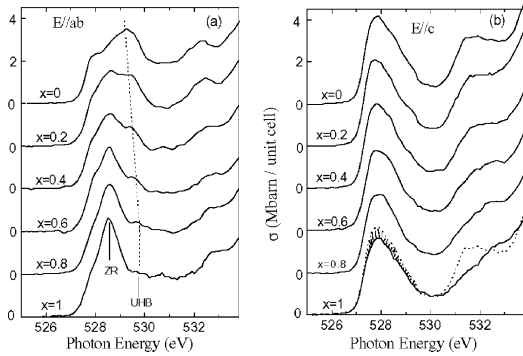


Fig. 1. Polarized O K-edge X-ray absorption spectra of the $Y_xPr_{1-x}Ba_2Cu_3O_7$ ($x = 0-1$) thin films for (a) $E||ab$ and (b) $E||c$ polarization. For comparison, the absorption spectrum of Pr123 is plotted as a dashed curve. The additional FR band is observed, as indicated by hatched lines.

Pr 4f–O 2p hybridized states or FR states. Fig. 1(b) presents the O K-edge X-ray absorption spectra of the $Y_xPr_{1-x}Ba_2Cu_3O_7$ ($x = 0-1$) thin films for $E||c$ polarization. For $YBa_2Cu_3O_7$, the absorption peak at ~ 527.8 eV is assigned to the O 2p_z hole states in the apical oxygen sites. Upon Pr substitution, an additional small band around 527.8–529.5 eV is observed. It is ascribed the additional spectral weight in the $E||c$ spectra of $Y_xPr_{1-x}Ba_2Cu_3O_7$ to the Pr 4f–O 2p hybridized states [5]. As noted, the energy of this band is in the same range as the ZR states observed for the $E||ab$ spectra below the UHB. Accordingly, the substitution of Y by Pr in $Y_xPr_{1-x}Ba_2Cu_3O_7$ induces a transfer of hole carriers from the ZR states to the energetically favored FR states, as evidenced in Fig. 1. The experimental results provide direct spectroscopic evidence in support of the FR model.

In Fig. 2(a), the O K-edge X-ray absorption spectra of the polycrystalline $Y_xPr_{1-x}Ba_2Cu_4O_8$ ($x = 0-1$) samples are presented. The pre-edge peak at ~ 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 ~ 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 ~ 529.6 eV is ascribed to the upper Hubbard Cu 3d conduction band. As noted from Fig. 2(a), the pre-edge peaks at ~ 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.

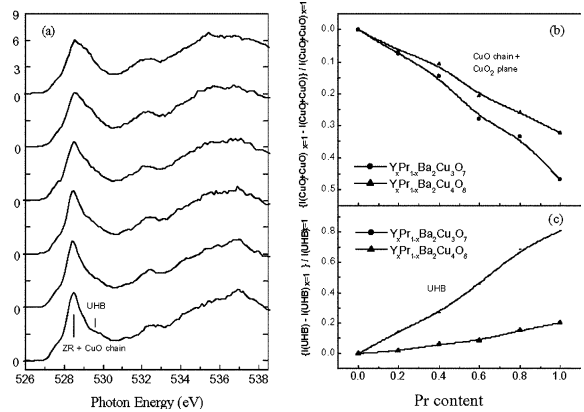


Fig. 2. (a) O K-edge X-ray absorption spectra of $Y_xPr_{1-x}Ba_2Cu_4O_8$ ($x = 0-1$). Variation rates of (b) hole carriers in the CuO_2 plane + CuO chain, and (c) spectral weight of the UHB for $Y_xPr_{1-x}Ba_2Cu_3O_7$ and $Y_xPr_{1-x}Ba_2Cu_4O_8$ relative to the undoped parent cuprates for $x = 1$.

Fig. 2 (b) and (c) present the change rates of hole carriers in the ZR states and CuO chains and spectral weight of the UHB for $Y_xPr_{1-x}Ba_2Cu_4O_8$ and $Y_xPr_{1-x}Ba_2Cu_3O_7$ relative to the undoped parent cuprates for $x = 1$. As noted from Fig. 2(b), upon Pr substitution, the reduction rate of hole carriers within the ZR states and CuO chains in $Y_xPr_{1-x}Ba_2Cu_4O_8$ is considerably slower than that in $Y_xPr_{1-x}Ba_2Cu_3O_7$. Moreover, the increased rate of spectral weight in the UHB with Pr doping in $Y_xPr_{1-x}Ba_2Cu_4O_8$ is significantly higher than that in $Y_xPr_{1-x}Ba_2Cu_3O_7$, as shown in Fig. 2(c). Thus, the T_c suppression rate with Pr doping in $Y_xPr_{1-x}Ba_2Cu_4O_8$ is slower than that in $Y_xPr_{1-x}Ba_2Cu_3O_7$.

In conclusion, we demonstrate spectroscopic evidence of the existence of FR states. Based on present X-ray absorption studies, the oxygen content affects the hole depletion rate of cuprates with Pr doping.

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