2C/2005G101

Spectral weight transfer in $Pr_{1-x}Ca_xMnO_3$ studied by photoemission spectroscopy

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Introduction

In recent decades, manganites have been extensively studied because of their remarkable physical properties such as colossal magnetoresistance (CMR) and spin, charge and orbital ordering. The compound $Pr_{1-x}Ca_xMnO_3$ (PCMO), in which the band-width W is small in comparison with other manganites, has a particularly stable charge ordered (CO) state [1]. Furthermore, CMR in the CO state of PCMO has been remarkable, amounting to several orders magnitude [1]. In this paper, we report on the composition dependence of the valence-band spectra in single crystals of PCMO.

Experimental

Single crystals of PCMO with the carrier concentrations of x = 0.2, 0.25, 0.3, 0.45, 0.5 and 0.65 were grown by the floating-zone method. The photoemission spectroscopy (PES) measurements were performed at BL-2C of Photon Factory, High Energy Accelerators Research Organization (KEK) using photon energy of $h\nu$ = 600 eV, 643.6 eV (Mn2*p*-3*d* resonance), 930 eV (Pr 3*d*-4*f* resonance). Ultraviolet photoemission spectroscopy (UPS) was also performed using the photon energy $h\nu$ = 21.2 eV. All the measurements were performed under the base pressure of ~10^{-10} Torr at room temperature. Clean surfaces were obtained by repeated *in situ* scraping with a diamond file.

Results and Discussion

Valence-band spectra of PCMO taken at different photon energies are shown in Fig. 1(a). The spectra mainly consisted of structures as labeled A, A', B, C, C', C", and D. The spectra taken at $h\nu$ = 930 eV and 643.6 eV correspond to Pr 3*d*-4*f* and Mn 2*p*-3*d* on-resonant PES spectra, respectively. From the Mn 2*p*-3*d* resonance spectra, Mn 3*d*-derived features appeared as structures A', C', and D. Structures A' and C' are shifted slightly toward higher binding energies than A and C, respectively, due to the different matrix elements between normal PES and resonant PES. Also, the intensity of structure C" was strongly enhanced in the Pr 3*d*-4*f* resonance spectra. The UPS ($h\nu$ = 21.2 eV) spectrum represents the O 2*p* state due to the large relative photo-ionization cross-section of O 2*p* at low photon energies. Therefore, structures A, B, C, and D in the UPS spectrum are assigned to the Mn 3*d*-O 2*p* bonding state, the non-bonding O 2*p* state, the Mn 3*d* t_{2g} plus the Pr 4*f* states, and the Mn 3*d* e_g state, respectively, consistent with the cluster-model calculation for $La_{1-x}Sr_xMnO_3$ (LSMO) [2].

Figure 1(b), 1(c) shows the valence-band spectra near Fermi level (E_F) for various hole concentrations taken at $h\nu$ = 21.2 eV and 600 eV, respectively. The spectra have been normalized to the integrated intensity in the energy range from 1.5 eV to ~E_F. Two features labeled D' and D" were observed in these spectra. Spectral weight was transferred from D' to D" with increasing hole concentration, that is, the valence-band spectra near E_F exhibited highly non-rigid-band-like behavior, similar to that in the LSMO [2].

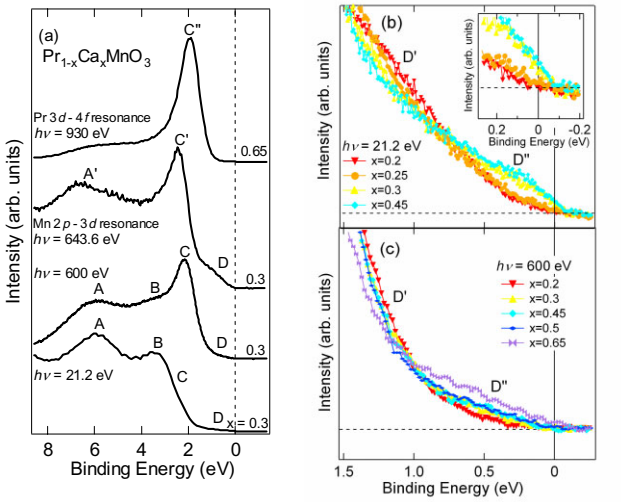

Fig. 1: Valence band photoemission spectra of $Pr_{1-x}Ca_xMnO_3$. (a) Comparison of spectra taken at various photon energies; (b) Spectra near E_F taken at $h\nu$ = 21.2 eV; (c) $h\nu$ = 600 eV.

References

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