Large Thermoelectric Power of Ca_{1-x}Na_xCo₂O₄ Studied by Soft-X-Ray Absorption Spectroscopy

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Transition-metal oxides are known to show various exotic phenomena such as high- T_c superconductivity and colossal magnetoresistance. Since the large thermoelectric power (LTP) of Na_xCo₂O₄ with a layered structure was discovered in 1997, enormous studies have been performed to reveal the possibly unconventional mechanism (1,2). Other cobalt oxide with a 3-dimentional crystal structure, Ca_{1-x}Na_xCo₂O₄, was recently reported to show comparable LTP, suggesting that the LTP and its mechanism may be in common in these cobalt oxides (3,4). To investigate the Co 3*d* electronic states that are expected to play an essential role for the LTP in Ca_{1-x}Na_xCo₂O₄, we have carried out the soft-x-ray absorption spectroscopy (SXAS).

The SXAS experiment was carried out at the BL-11 of the SR center in Ritsumeikan University. The spectra were recorded by the total electron yield (TEY), partial electron yield (PEY), partial fluorescence yield (PFY), and inverse partial fluorescence yield (IPFY) methods at the room temperature.

Figure 1 shows the O *K*-edge absorption spectra of $Ca_{1-x}Na_xCo_2O_4$ (x=0 and 0.5). Holes are found to be doped in Co 3*d* t_{2g} bands by the sodium substitution. The variation of O *K*-edge absorption spectrum due to the substitution seems to be explained within the rigid-band picture as seen in the Co 3*d* partial density of states (PDOS) calculated on the basis of the density functional theory. Meanwhile, only a slight difference was observed between x=0 and 0.5 in the Co $L_{2,3}$ -edge absorption spectrum as shown in Fig. 2.

References

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Fig. 1 O *K*-edge absorption spectra of Ca_{1-x} Na_xCo₂O₄ (*x*=0, 0.5) measured by the PFY method. Ca *d*-, Co *d*-, and O *p*-state PDOSs of CaCo₂O₄ are also shown.



Fig. 2 Co $L_{2,3}$ -edge absorption spectra of Ca_{1-x}Na_xCo₂O₄ (x=0, 0.5) measured by PEY and IPFY methods. The spectra are normalized by the L_3 -peak intensity after subtracting backgrounds.