BS06

Electronic Structure, Spin States, and Thermoelectric Power of Low Dimensional Cobaltates $Ca_3Co_4O_9$ and $Ca_3Co_2O_6$

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Recently, cobalt oxides with a low dimensional structure such as Na_xCoO_2, $Ca_3Co_4O_9$, $Ca_3Co_2O_6$, etc. have attracted much attention due to the discovery of their large thermoelectric power of ~100 μV/K [1-3]. Interestingly, these cobaltates show several common features such as low dimensional structure, low electric conductivity, and the suspected mixed-valency of the cobalt ions. To understand the origin of the large thermoelectric power, roughly two approaches have been tried. One is the entropy approach that applies the Heikes formula to the spin-degeneracy of the cobalt ions in the Hubbard model for the strongly correlated electron systems [4], and the other is the traditional approach in which the thermoelectric power is calculated from the density of the states near the Fermi level under the relaxation time approximation. Many experimental studies have reported that the application of the Heikes formula is not appropriate for the cobaltates, though the spin degeneracy may play a role in part. In order to investigate the origin of the large thermoelectric power of the cobaltates and clarify this issue, we have performed x-ray absorption spectroscopy and photoelectron spectroscopy on the quasi-1 dimensional $Ca_3Co_2O_6$ and quasi-2 dimensional misfit-layered $Ca_3Co_4O_9$ using synchrotron radiation facilities. By combining the Co 2*p* photoelectron spectra, Co 2*p* absorption spectra, and O 1s absorption spectra, we obtained valence states and spin states of the Co ions. Additionally we extracted the several important parameters for the electronic structure of the cobaltates using configuration interaction cluster model calculation, and checked the pre-requisites for the Heikes formula.

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BS07

Magnetic Property of $Bi_xCa_{1-x}MnO_3$: Experimental and First Principle Calculation Study

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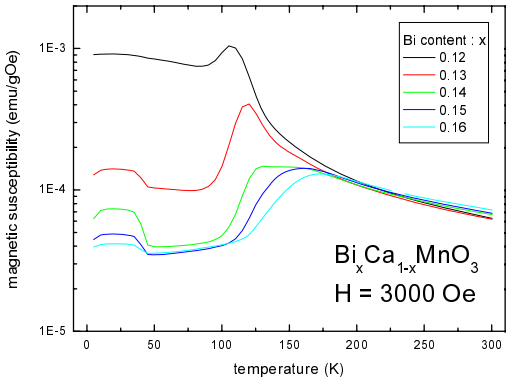
Magnetic property of $Bi_xCa_{1-x}MnO_3$ for x = 0.12, 0.13, 0.14, 0.15, and 0.16 are investigated by the measurement and analysis of their magnetic susceptibility, resistivity, and electron magnetic resonance at different temperatures. As is formerly known (see [1]-[3]), $Bi_xCa_{1-x}MnO_3$ shows quite the complicated magnetic and crystal structure transitions with the temperature and composition changes – particularly for Bi composition x is near 0.15. It is the main purpose of our experiments to clearly see how the magnetic properties and resistivity of $Bi_xCa_{1-x}MnO_3$ change in this region. And the underlying mechanisms involved are discussed.



Also the first principle calculations about the magnetic phase of $Bi_xCa_{1-x}MnO_3$ for x = 0, 0.25, 0.5, 0.75, and 1 are carried and the results – the spin state, electric and magnetic characters are analyzed.

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