An Electron Momentum Density Analysis for Spin Crossover Materials

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Cobalt oxides are one of the fundamentally interesting and technologically important materials because of their multiple degree of freedoms on spin, charge and lattice. Not only to lithium ion batteries, but also to fuel cells, thermoelectric conversion devices and superconductivity applications, the fascinating oxides possess a wide range of capabilities. One of the central issues in these materials is the spin crossover phenomena in $LaCoO_3$, in which two step anomalies are observed in magnetism and transport at ~100 K and ~500 K. Based on a model of Co^{3+} with d^6 configuration, the transition from low spin (LS: t_{2g}^6) to high spin (HS: $t_{2g}^4 e_g^2$), via possible intermediate spin (IS: $t_{2g}^5 e_g^1$) (see Fig.1), has been intensively studied [1].

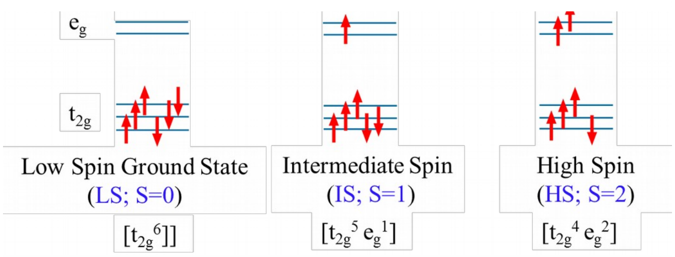

Fig.1 Spin states in d^6 configuration.

In this work we have carried out X-ray Compton scattering experiment on single-crystalline $LaCoO_3$ to reveal the evolving character of the electronic states associated with the spin crossover phenomena. Two-dimensional electron momentum density (2D-EMD) distributions at 10 K and room temperature were reconstructed from seven measured Compton profiles, and the difference 2D-EMD distribution was obtained (see Fig.2). The results are in excellent accord with the electron transfer from the t_{2g} state to the e_g state for the spin transition, and significant hybridization of e_g with ligand O 2*p* is obviously observed. In this presentation, we also present latest progress.

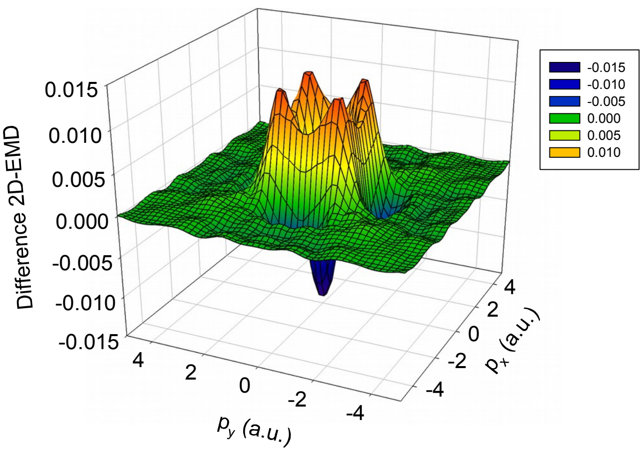

Fig.2 Difference 2D-EMD distribution between 10 K and RT.

Reference:

[1] K. Asai *et al.*, J. Phys. Soc. Jpn. **67** (1998) 290.