Electronic Structure of the $La_{5/3}Sr_{1/3}NiO_4$ Studied by X-ray Absorption Spectroscopy

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$La_{5/3}Sr_{1/3}NiO_4$ is a model system for studying strong electron-phonon coupling, it displays no structural phase transtions at low temperatures but strong effects of charge ordering at $T_C \approx 240$ K and spin ordering at $T_N \approx 190$ K in real space [1]. La substitution by Sr or excess oxygen provide hole carries into the NiO_2 planes and coupled charge or spin modulations start to form. In particular, it shows a metallic behavior only at a very high doping level and do not exhibit a superconducting transition, unlike the isostructural La_2CuO_4.

In this respect, angle dependent X-ray absorption near-edge structures (XANES) spectroscopy were performed at the wiggler-17C (Ni *K*-edge) and 16A (La *L*-edge) beamlines of National Synchrotron Radiation Research Center in Hsinchu, Taiwan. All data were obtained in fluorescence mode at room temperature.

Angle dependent Ni *K*-edge spectra were measured for a single crystal, where spectra at the $\theta_i = 0^o$ and 70^o, approximately correspond to those for x-ray polarization vector ε parallel to the *c* axis ($\varepsilon \| c$) and to the *ab* plane ($\varepsilon \perp c$), respectively.

Ni *K*-edge XANES shows that the overall spectral feature shifts to higher energies, indicating the imbalance of charge states between in-plane (Ni^{3+}, hole dominant) and out-plane (Ni^{2+}, hole deficient) of Ni-O octahedra. This fact is well consistent with the previous results of polarized spectra [2]. Pre-edge peak in the inset, which is assigned to $1s \rightarrow 3d$ quadrupole transition, also shifts to higher energies.

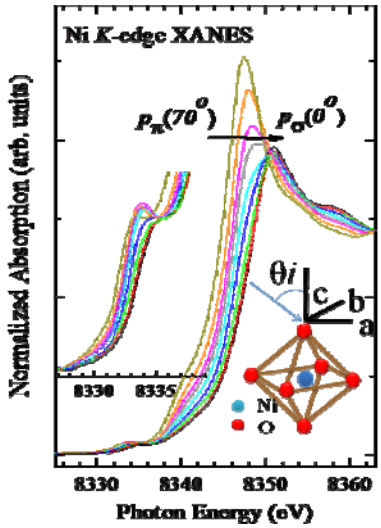

Fig. 1: Angel dependence of Ni *K*-edge XANES. Inset shows the pre-edge related to the Ni $1s \rightarrow 3d$ quadrupole transition.

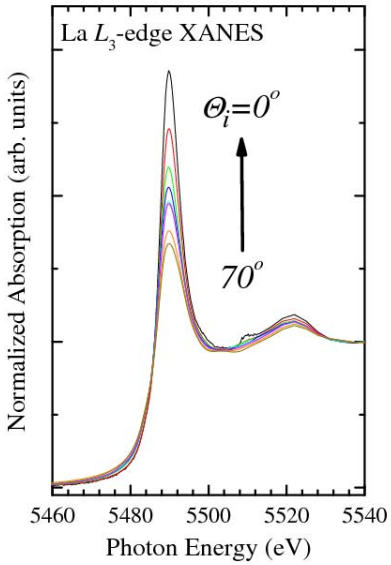

Fig. 2: Angel dependence of Ni *K*-edge XANES.

In La L_3-edge XANES, there is no energy shift except the intensity variation, which is proportional to the hole density of unoccupied states.

The angle dependence of Ni *K*- and La *L*-edge XANES presents the continuous evolution of spectra upon the oxidation states of Ni or hole density of La, in which Ni and La atoms are bonded with oxygen. Consequently it is clear that the doped holes in the present nickelates are preferentially located ab plane. The diagonal direction to Ni-O bond is revealed to have the commensurable charge distribution.

References

[1] C. H. Chen *et al.*, Phys. Rev. Lett. **71**, 2461 (1993).
[2] A. Sahiner *et al.*, Phys. Rev. B **51**, 5879 (1995).