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Electronic structure study of $Li_xNi_{1-x}O$ epitaxial thin films

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Recently, large amount of Li doped NiO epitaxial thin films were successfully grown on sapphire (0001) substrates with a (111) orientation by a room-temperature pulsed laser deposition method [1]. These Li-Ni-O thin films are potential materials for various applications, such as electrochromic devices, UV detectors, and gas sensors [2].

Hard x-ray photoelectron spectroscopy (HAXPES) has been used to study the electronic structures of cubic-phase $Li_xNi_{1-x}O$ epitaxial thin films with lithium component of x = 0, 0.27, and 0.48. The HAXPES experiments were performed with photon energy of 5.95 keV at the undulator beamline BL15XU of SPring-8, Japan.

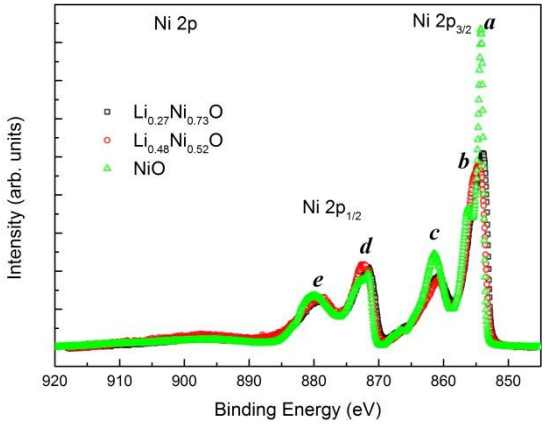

Figure 1: Ni 2*p* HAXPES spectra

As shown in figure 1, we discussed three distinct *a*, *b* and *c* features observed in the Ni $2p_{3/2}$ core-level spectra using an extended configuration interaction model including the Zhang-Rice doublet bound state. The area ratio result indicates that the Zhang-Rice doublet bound state decrease by the Li substitution at Ni site in NiO. The reduction of the Zhang-Rice state results in the hole injection in the top of the valence band.

The valence band spectra of $Li_xNi_{1-x}O$ thin films consist of some peaks such as *A*, *B*, *C*, *D*, *E*, *F*, and *G*. Furthermore, *F* and *G* peak intensities seemed considerably strong at x = 0.48. The *A* and *B* features origin from $\underline{Z}$ hole in ZR doublet bound state, feature *C* and *D* from $\underline{L}$ hole in ligand state, respectively [3]. These valence band structures can be assigned as *A* and *B* to $3d^8\underline{Z}$, where $\underline{Z}$ is a hole in bound state of neighboring Ni atoms. In addition, the structures *C* and *D* have been assigned to mixture of $3d^7$ and $3d^8\underline{L}$ configurations, where $\underline{L}$ is a hole in ligand states of O 2*p* band.

In this study, the observed core-level and valence band spectra are well interpreted by an extended configuration interaction model including the Zhang-Rice doublet bound state.

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[2]. H. Ohta et al. Appl. Phys. Lett. **83**, 1029 (2003).

[3]. M. Taguchi et al. Phys. Rev. Lett. **100**, 206401 (2008)