Hard X-ray photoelectron spectroscopy of epitaxially grown $M_xNi_{1-x}O$ (M = Li, Mg)

NIMS/SPring-8 [1], Tokyo Tech. [2], NAIST [3]

◦L. S. R. Kumara[1], Anli Yang[1], Osami Sakata[1,2], Ryosuke Yamauchi[2], Munetaka Taguchi[3], Satoshi Ishimaru[1], Akifumi Matsuda[2], and Mamoru Yoshimoto[2]

E-mail: KUMARA.Rosantha@nims.go.jp

Recently, nickel-based cathodes have much interest in advanced technology applications as electrode materials. In rechargeable lithium batteries, nickel is employed in the form of oxide in which lithium ions are intercalated into its crystal structure to form the layered nickel oxide. When Li^+ is partially substitute the normal site of Ni^{2+}, a hole is introduced in the form of Ni^{3+} or O^- to keep charge neutrality conditions, and the oxide becomes a black semiconductor [1].

In addition, $Mg_xNi_{1-x}O$ epitaxial thin films were grown on sapphire (0001) substrates using PLD to stabilize NiO nanosheets/graphene for lithium storages. On the other hand, the Mg fraction in $Mg_xNi_{1-x}O$ thin films did not affect the structural properties of the NiO based thin films [2]. Hard x-ray photoelectron spectroscopy (HAXPES) is powerful tool to study the electronic structure of strongly correlated system. The core-level and valence band spectra of $M_xNi_{1-x}O$ (M = Li, Mg) were obtained at the undulator beamline BL15XU of SPring-8 [3].

The three distinct features observed in the Ni $2p_{3/2}$ core-level spectra with increasing Li substitution were explained by the using an extended configuration interaction (CI) model including the Zhang-Rice doublet bound state [4]. The Ni 2*p* core-level spectra measured from $Mg_xNi_{1-x}O$ thin films are identical to that of NiO epitaxial thin films.

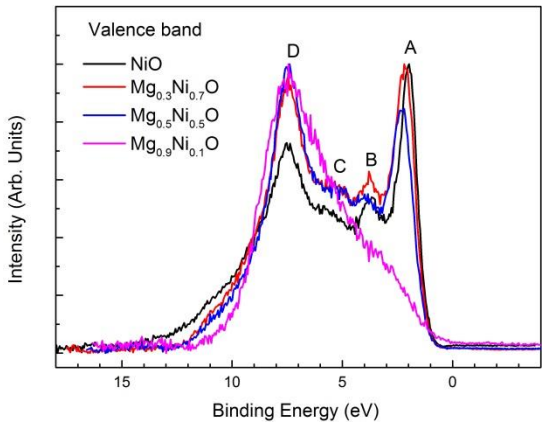

Figure 1: HAXPES valence band spectra epitaxially grown $Mg_xNi_{1-x}O$.

As shown in Figure 1, the valence band spectra of $Mg_xNi_{1-x}O$ thin films consist of four peaks labeled as *A*, *B*, *C*, and *D*, and the intensity of *A* and *B* peaks clearly decreased with increasing of the Mg content.

In this study, the electronic structure of $M_xNi_{1-x}O$ (M = Li, Mg) thin films were observed by analyzing their core-level and valence band HAXPES spectra, and interpreted using an extended CI model.

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(3) S. Ueda, J. Electron Spectrosc. Relat. Phenom. 190 (2013) 235

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