

# Electronic structure of $\text{Mn}_3\text{Cu}_{1-x}\text{Ga}_x\text{N}$ studied by soft X-ray photoelectron spectroscopy

Y. Miyata<sup>1</sup>, K. Mima<sup>1</sup>, R. Yamaguchi<sup>1</sup>, A. Yamasaki<sup>2</sup>, A. Higashiya<sup>3</sup>, T. Muro<sup>4</sup>,

K. Terashima<sup>1</sup>, K. Takenaka<sup>5</sup>, A. Ozawa<sup>5</sup>, T. Inagaki<sup>5</sup>, S. Imada<sup>1</sup>

<sup>1</sup> *Department of Physics, Ritsumeikan University, Kusatsu, Shiga 525-8577, Japan.*

<sup>2</sup> *Department of Physics, Faculty of Science and Engineering, Konan University, Kobe 658-8501, Japan*

<sup>3</sup> *SPring-8 / RIKEN, Hyogo 679-5148, Japan*

<sup>4</sup> *JASRI, SPring-8, Hyogo 679-5198, Japan*

<sup>5</sup> *Department of Crystalline Materials Science, Nagoya University, Nagoya 464-8603, Japan*

Antiperovskite manganese nitrides  $\text{Mn}_3\text{XN}$  ( $\text{A}=\text{Zn}$ ,  $\text{Ga}$ , etc) are potential candidates for large negative thermal expansion (NTE) materials. These nitrides are well known for their large magnetovolume effect (MVE) [1]. Unlike other  $\text{Mn}_3\text{XN}$ ,  $\text{Mn}_3\text{CuN}$  does not show MVE. Instead,  $\text{Mn}_3\text{CuN}$  undergoes a first-order transition from the high-temperature paramagnetic to the low-temperature ferromagnetic phase at  $T_C=143\text{K}$ , accompanied by cubic-to-tetragonal structural deformation [2].

In order to clarify the relationship between crystal structure and magnetic structure in this system, we studied the electronic states of  $\text{Mn}_3\text{Cu}_{1-x}\text{Ga}_x\text{N}$  by soft X-ray photoelectron spectroscopy (SXPES). We have also carried out band structure calculation, and compared the obtained electronic structures with the experimental results. Figure 1 shows the valence band SXPES spectra of  $\text{Mn}_3\text{CuN}$  and  $\text{Mn}_3\text{Cu}_{0.5}\text{Ga}_{0.5}\text{N}$ , the latter showing MVE, measured with the incident photon energy of 700 eV. Both spectra consists of three characteristic structures; a peak in the vicinity of Fermi level, a peak at 3.5 eV, and a hump at  $\sim 8$  eV. From the comparison between the SXPES result and band calculation, we identify each as mainly N 2p, Cu 3d, and Mn 3d bands, respectively. Next we compared the electronic states of  $\text{Mn}_3\text{Cu}_{0.5}\text{Ga}_{0.5}\text{N}$  with  $\text{Mn}_3\text{CuN}$ . Through the substitution of Ga for Cu, the photoelectron intensity peak at 3.5 eV decreases, whereas the peak in the vicinity of Fermi level becomes sharper. These changes are consistent with the results of the band calculation.

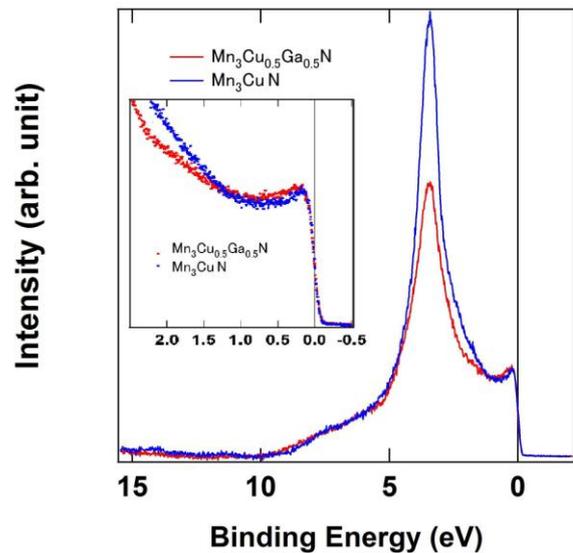


Fig. 1. SXPES spectra of  $\text{Mn}_3\text{CuN}$  and  $\text{Mn}_3\text{Cu}_{0.5}\text{Ga}_{0.5}\text{N}$ . In the main panel, the lines represent the spectra measured at 170K (paramagnetic phase), respectively. These spectra are normalized by the integrated intensity. The inset shows the magnified view of the spectra near the Fermi level where the red filled circles and the blue filled circles represent the spectra in  $\text{Mn}_3\text{CuN}$  and  $\text{Mn}_3\text{Cu}_{0.5}\text{Ga}_{0.5}\text{N}$  respectively.

[1] K. Takenaka *et al.*, Appl. Phys. Lett. **87** 261902 (2008)

[2] K. Takenaka *et al.*, Appl. Phys. Lett. **92** 161909 (2008)