SPECTROSCOPIC STUDY OF Ni-RICH Al-Co-Ni QUASICRYSTAL

K. Soda[1], M. Inukai[2], M. Kato[1], S. Yagi[1], Y. G. So[3], and K. Edagawa[3]

[1] *Graduate School of Engineering, Nagoya University, Nagoya 464-8603, Japan*
[2] *Venture Business Laboratory, Nagoya University, Nagoya 464-8603, Japan*
[3] *Institute of Industrial Science, The University of Tokyo, Tokyo 153-8505, Japan*

Various structural modifications have been found as a function of the Co/Ni ratio in decagonal Al-Co-Ni quasicrystals (QC) by electron microscopy [1]. However, it is still hard to distinguish Co from Ni in the microscopic image. Thus, in order to clarify the chemical nature bringing the unique atomic arrangement with the various modifications, we have studied the transition metal arrangement by comparing the electronic structures obtained by spectroscopic observation and model cluster calculation [2,3]. In this study, we report the results of soft x-ray photoelectron spectroscopy (XPS) and discrete variational $X\alpha$ (DV-$X\alpha$) cluster calculation for a Ni-rich Al-Co-Ni QC.

In Fig.1, a typical XPS spectrum of the Ni-rich QC is compared with that of a Co-rich one and the electronic density of states (DOS) derived from a Ni-rich model cluster shown in Fig.2. Here, the model cluster is based on a theoretical prediction with use of the interatomic pair potential [4], which shows a Ni-Ni interaction as well as a strong Al-Co one. The present cluster calculation also predicts bimodal Ni partial DOS consisting of the Ni-Ni bonding and anti-bonding bands. However, the XPS spectrum of the Ni-rich QC is peaked at higher binding energy than the Co-rich one and seems not to show the predicted large anti-bonding component.

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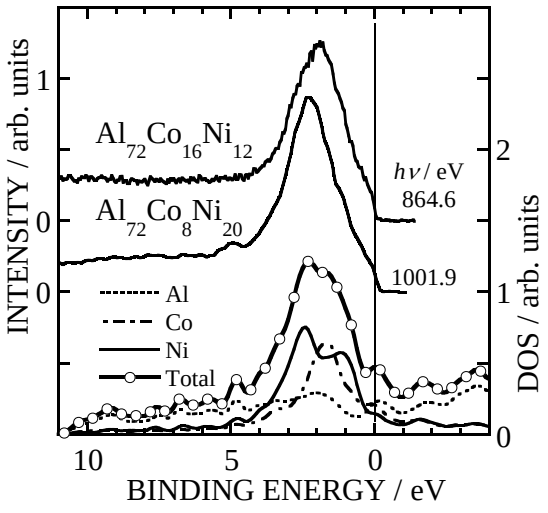

Fig.1 Photoelectron spectra and calculated density of states of Ni-rich Al-Co-Ni.

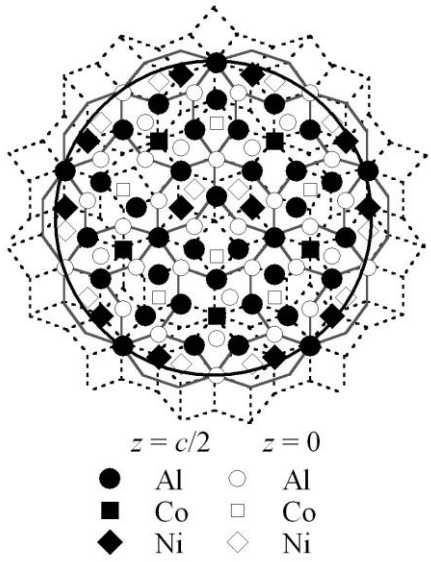

Fig.2 Cluster model of Ni-rich Al-Co-Ni.