2C/2010G189

Electronic Structure and Local Atomic Arrangement in 2-dimensional Quasicrystals Al-Co-Ni

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1 Introduction

Decagonal quasicrystals (d-QC), where quasiperiodic atomic layers are periodically stacked along a direction, are viewed as consisting of quasiperiodically arranged decagonal columnar structures. In particular, Al-Co-Ni alloys form d-QC in a wide concentration range with different structural modifications depending on a Co/Ni ratio [1]. According to a theoretical study [2], because of strong Al-Co and Ni-Ni interactions, a decagonal (pentagonal) ring of Al and transition metals (TM) are formed in the center of the column in Co-rich $Al_{72}Co_{20}Ni_8$, while Ni-rich $Al_{72}Co_8Ni_{20}$ shows an atomic arrangement in a hexagon-boat-star tiling with Ni-Ni pairs. However, it is difficult to distinguish these TM's by transition electron microscope. Thus we have investigated the electronic structures of Al-Co-Ni d-QC by the TM $L\alpha$ soft X-ray emission spectroscopy (XES) as well as the X-ray photoelectron one (XPS) and a cluster calculation in order to clarify the atomic arrangement from spectroscopic points of view.

2 Experiment

XES measurements were performed at BL2C of Photon Factory. The synchrotron light from the beamline was employed as the excitation source and its photon energy was calibrated by measuring XPS spectra of an Au plate. The energy of emitted photon was calibrated with the already calibrated and elastically scattered excitation photons. The energy resolution was estimated with the elastically scattered photons as ~1eV. Specimens were prepared by Ar arc-melting and subsequent quenching for Ni-rich d-QC $Al_{72}Co_8Ni_{20}$ and by the Czochralski method for Co-rich one $Al_{72}Co_{16}Ni_{12}$. They were mechanically polished before the XES measurement.

3 Results and Discussion

Figure 1 compares XES spectra of $Al_{72}Co_8Ni_{20}$ with those of $Al_{72}Co_{16}Ni_{12}$. In the figure, these XES spectra are plotted so that the integrated intensity is proportional to the TM concentration. While the 3*d* band in the XPS spectra, which represent the total electronic density of states (DOS), is shifted from the binding energy E_B of 2.3 eV in the Ni-rich d-QC to 1.8 eV in the Co-rich one, the spectral shape and peak position of the Co and Ni $L\alpha$ XES spectra, which stand for the partial DOS of the respective 3*d* states, in the Ni-rich d-QC are not so much different from those in the Co-rich one. In particular, a double peak feature predicted as a bonding and anti-bonding bands of the Ni-Ni pair in the Ni-rich d-QC by the electronic structure calculation for a model cluster (shown in the bottom panel of the figure) [3], is not recognized in the Ni $L\alpha$ XES spectrum. This is partly due to the emphasized Ni-Ni pairs in the model calculation and suggests the predominance of Ni-Al pairs or a strong Ni-Al interaction. This might also imply that the d-QC form as a TM atom is surrounded by Al atoms.

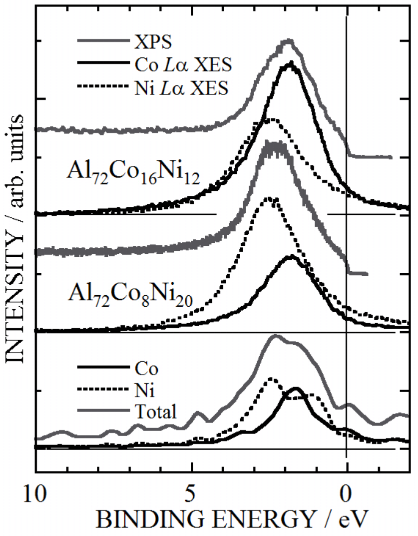

Fig. 1: XES and XPS spectra of Al-Co-Ni quasicrystals.

References
[1] S. Ritsch *et al.*, Phil. Mag. A **71** (1995) 671.
[2] S. Hiramatsu and Y. Ishii, J. Phys. Soc. Jpn. **75** (2006) 054602.
[3] K. Soda et al., Phil. Mag. **91** (2010) 2510.

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